

FIG. 1(a)

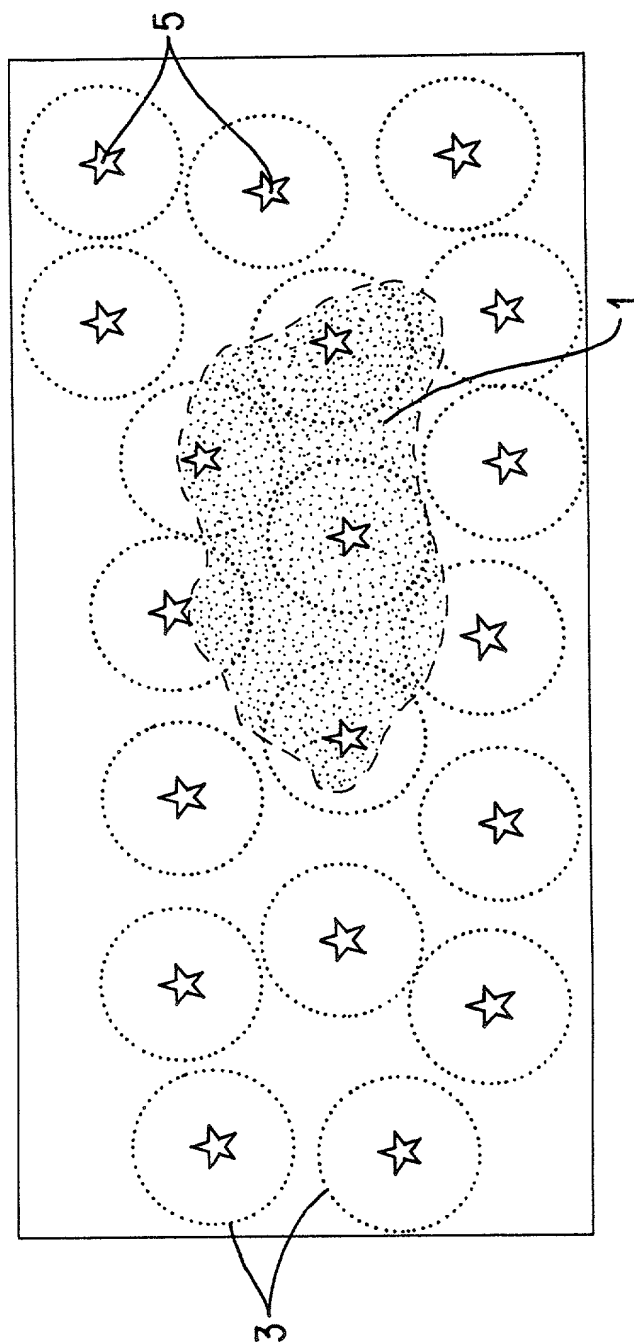


FIG. 1(b)

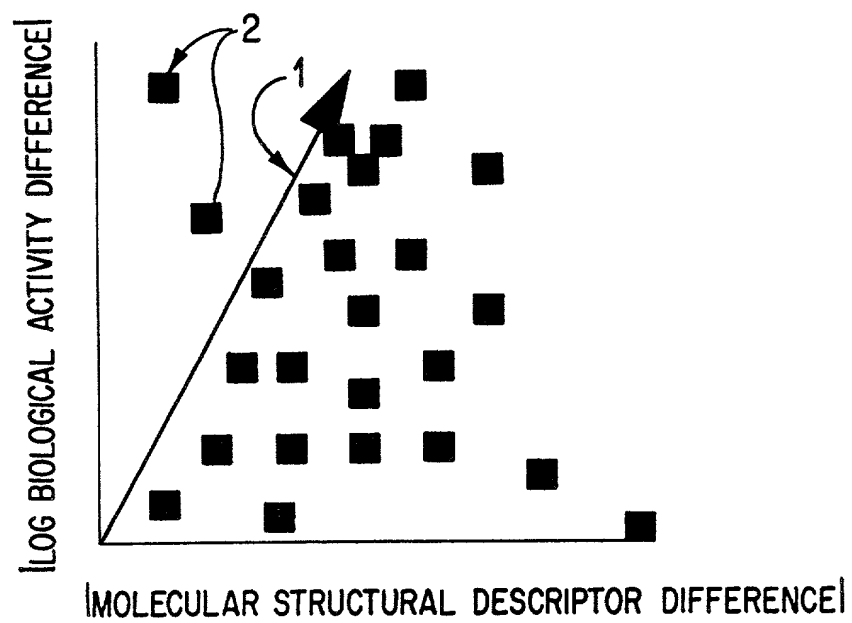


FIG. 2

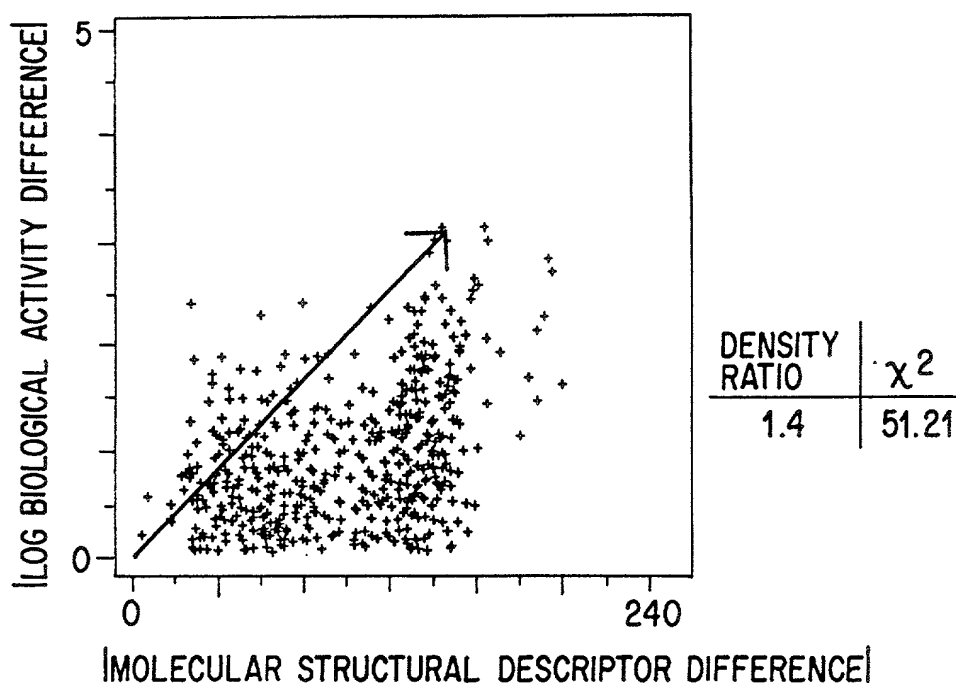


FIG. 3

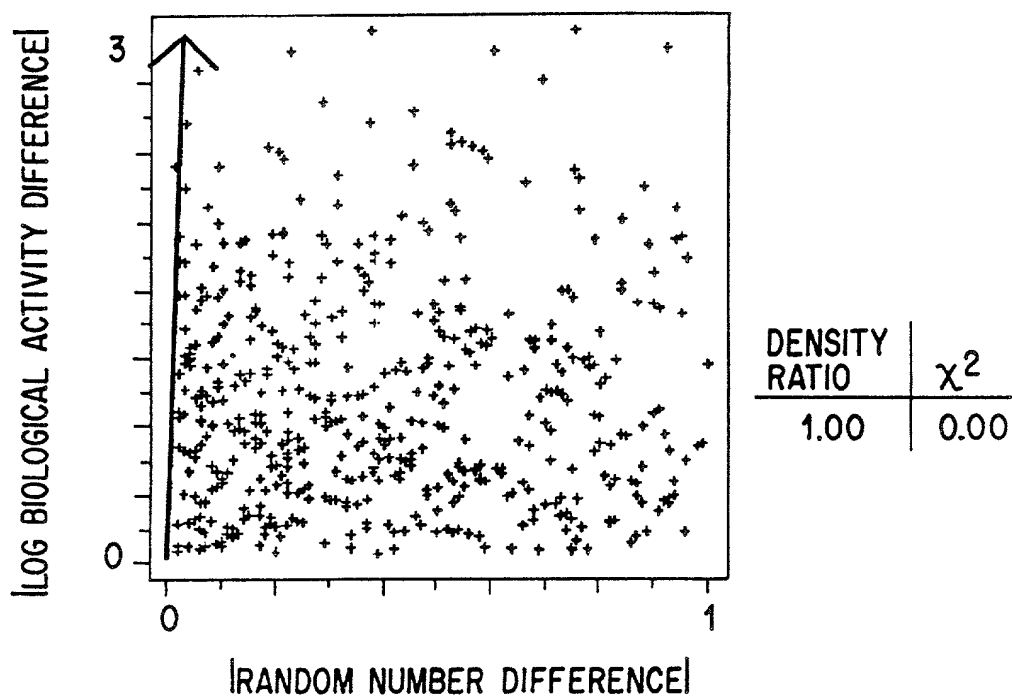


FIG. 4

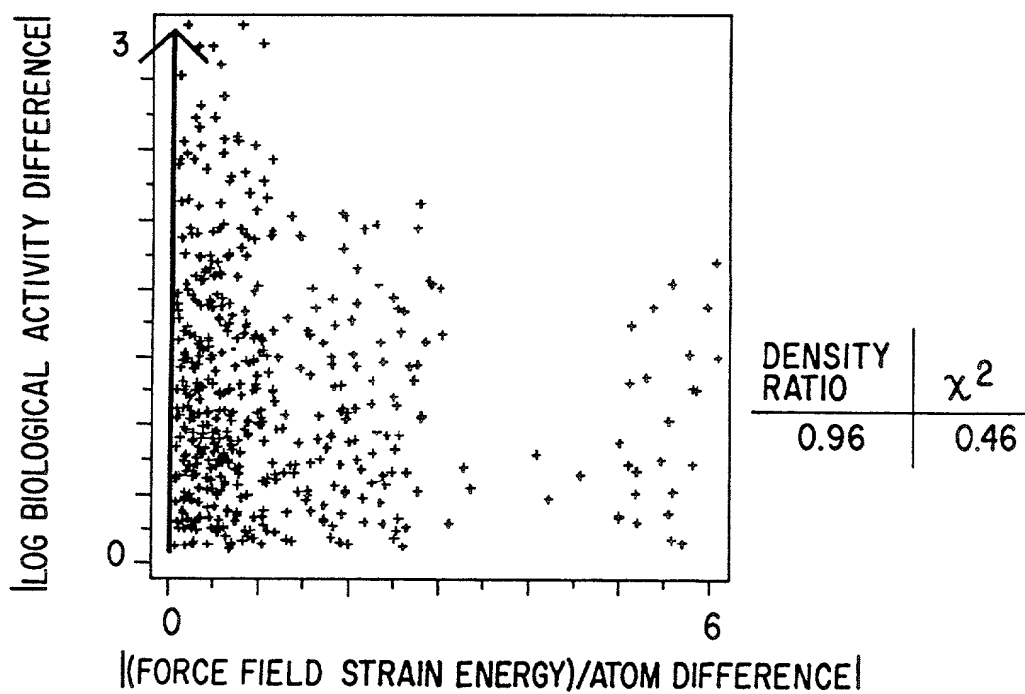
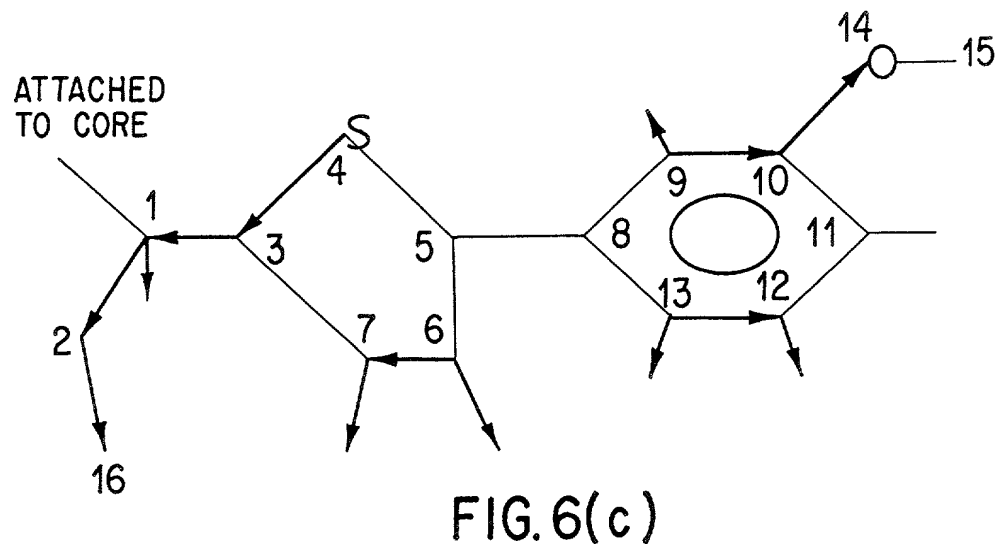
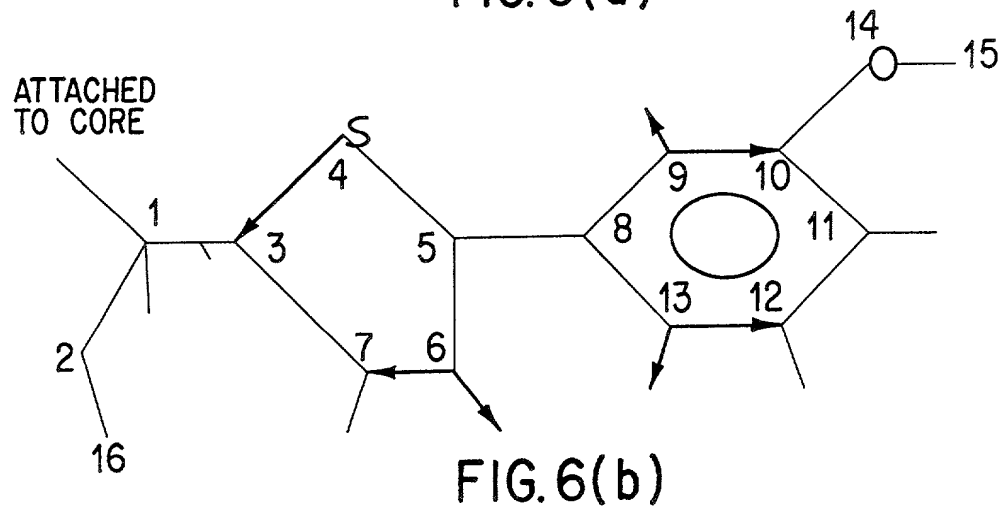
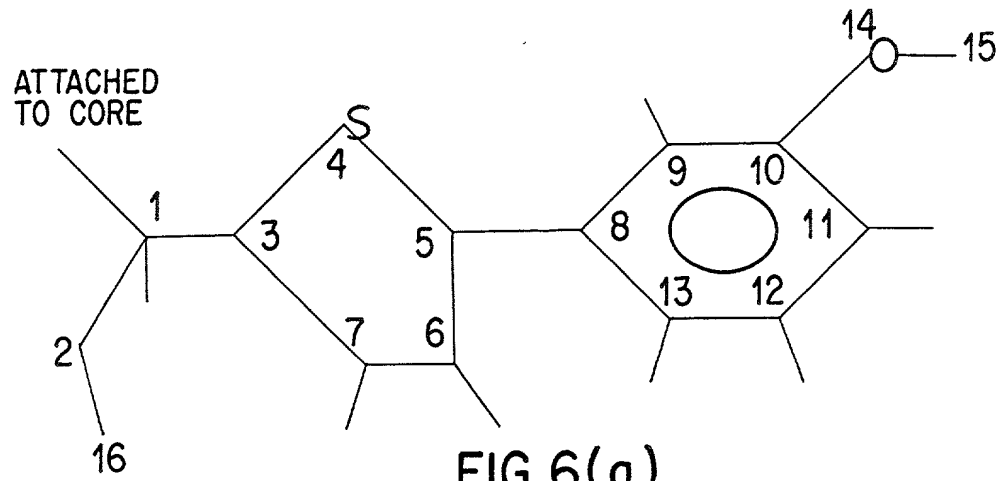


FIG. 5



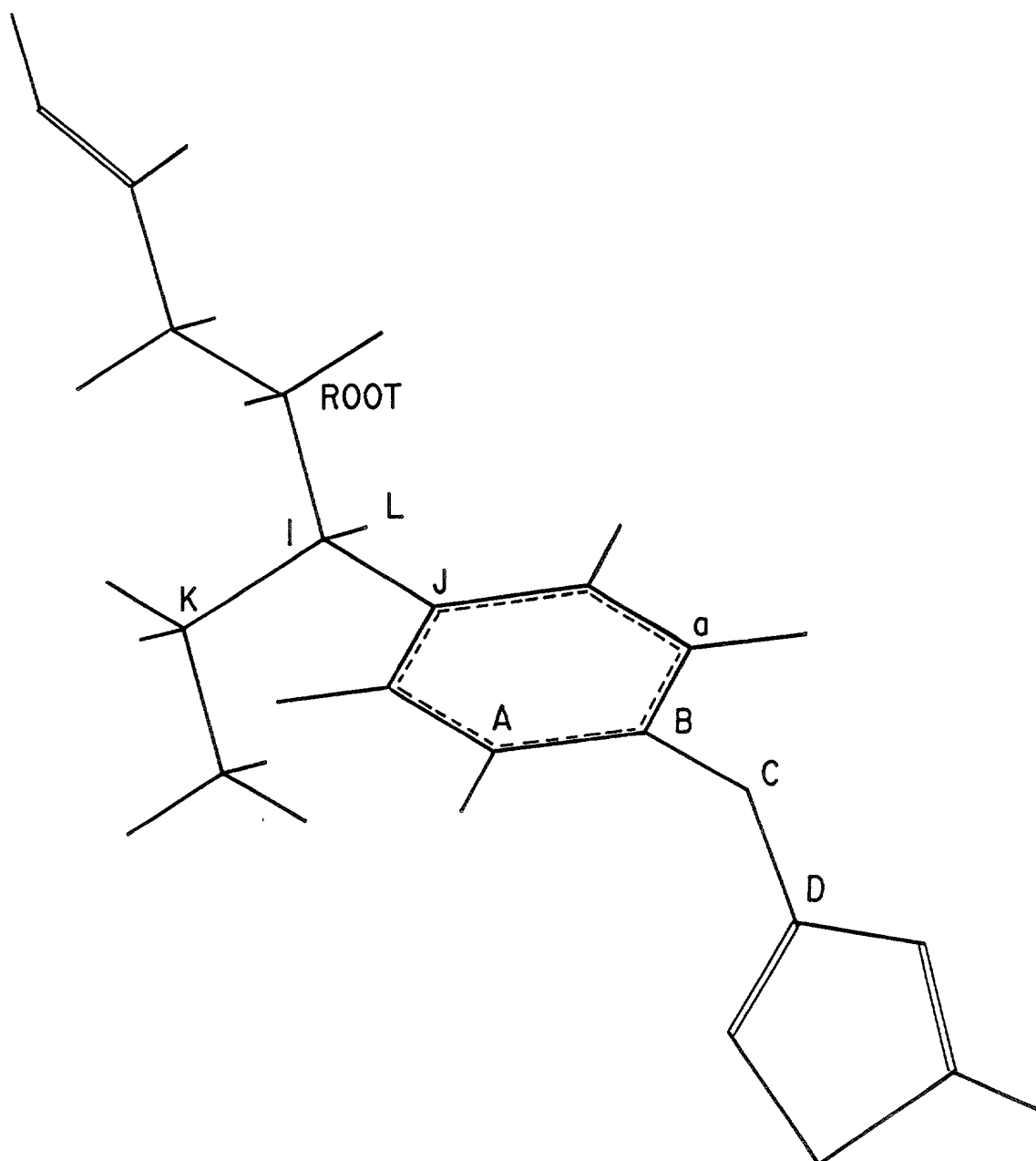


FIG. 6(d)

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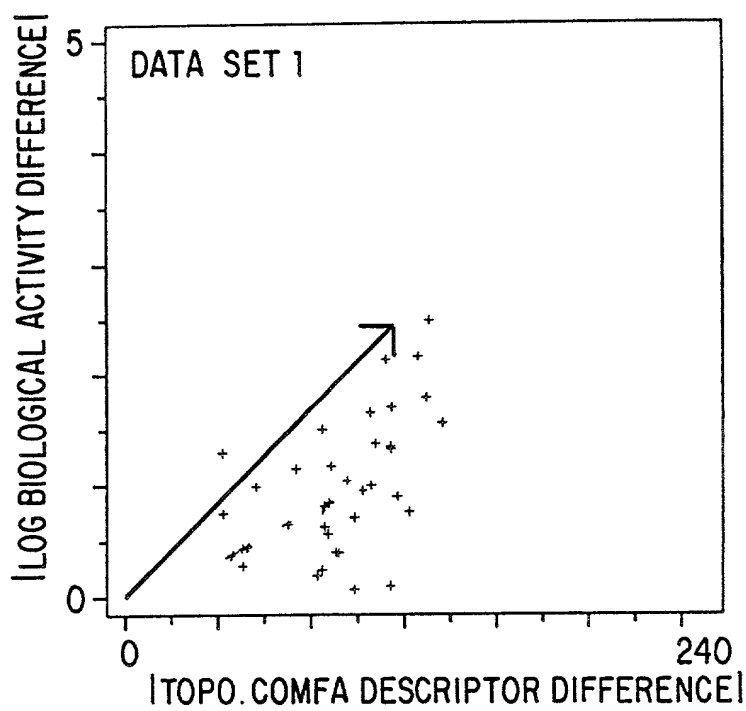


FIG.7(a)

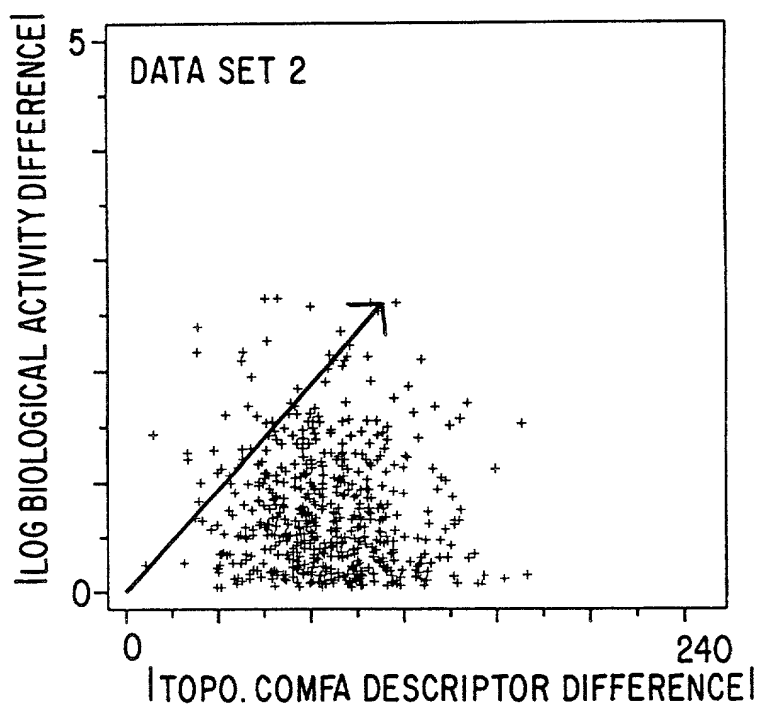


FIG.7(b)

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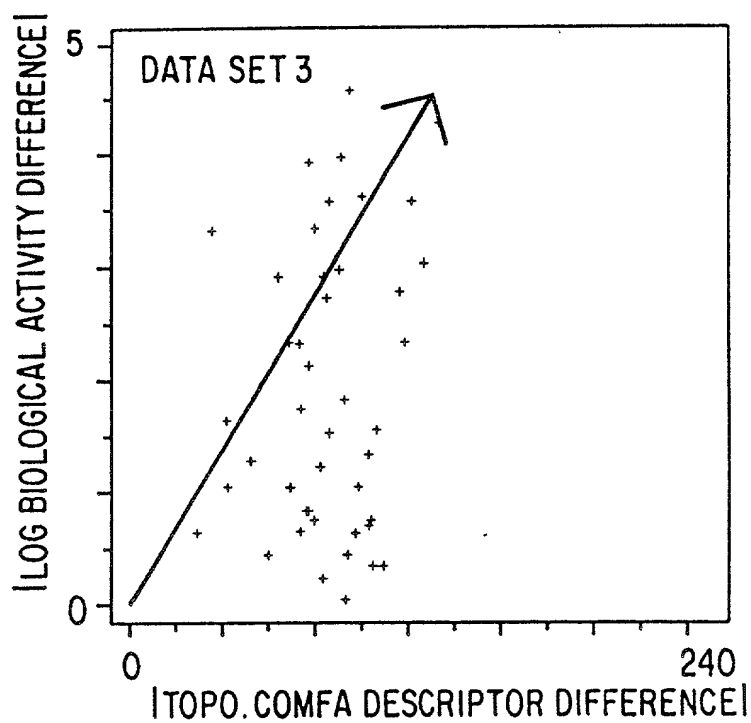


FIG. 7(c)

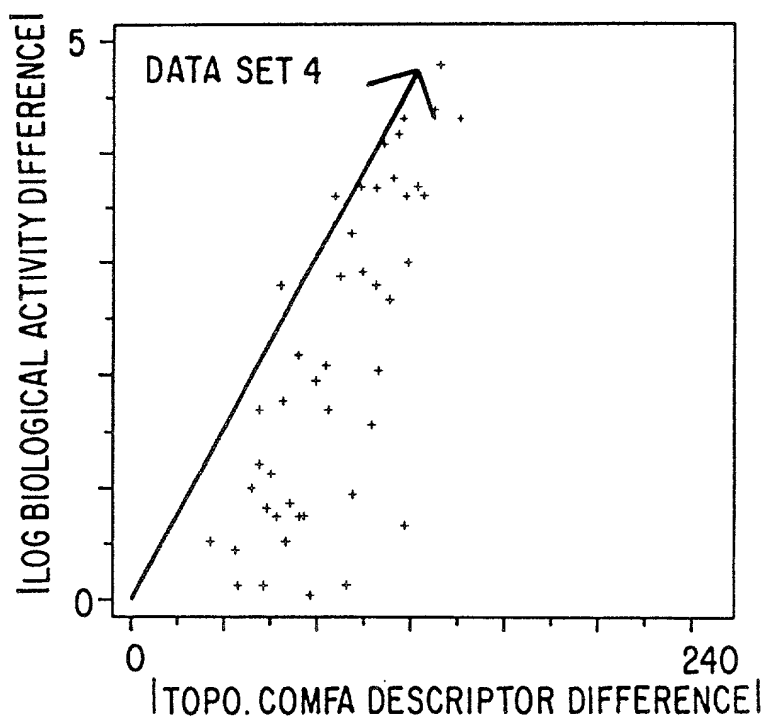


FIG. 7(d)

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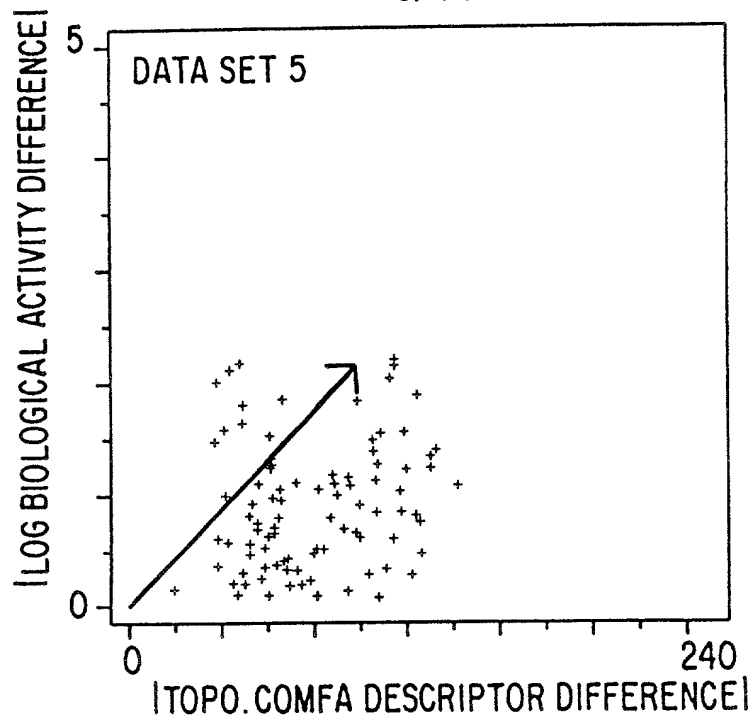


FIG.7(e)

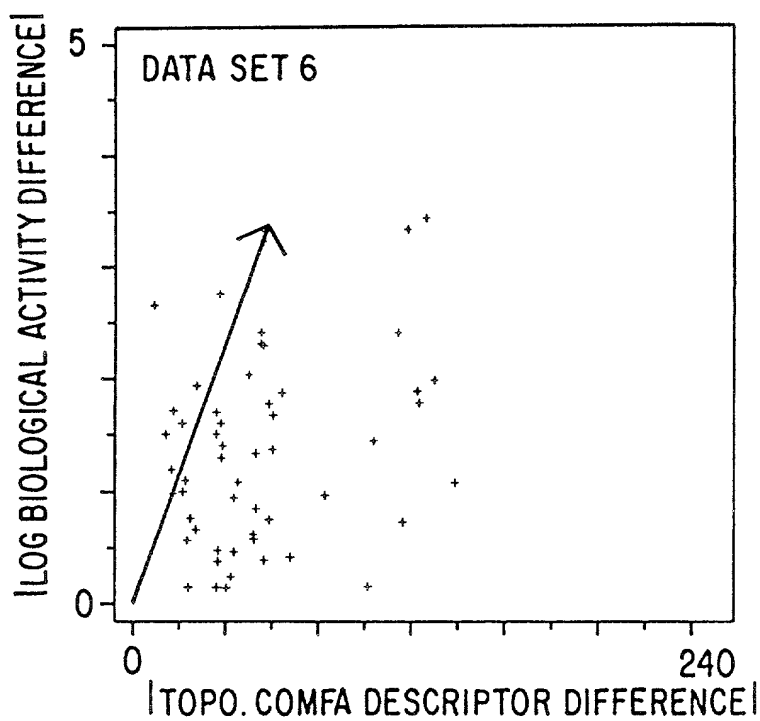


FIG.7(f)

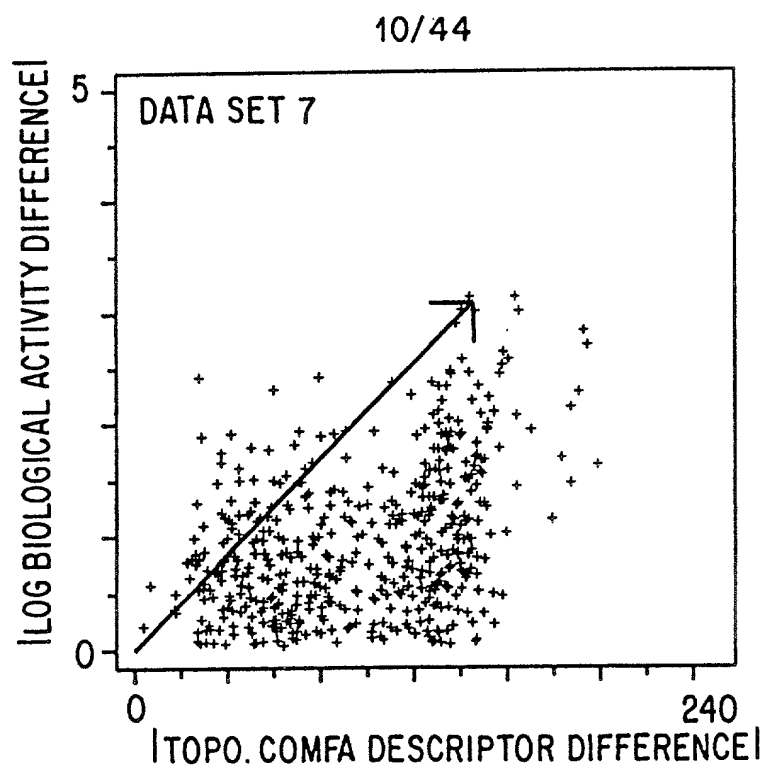


FIG.7(g)

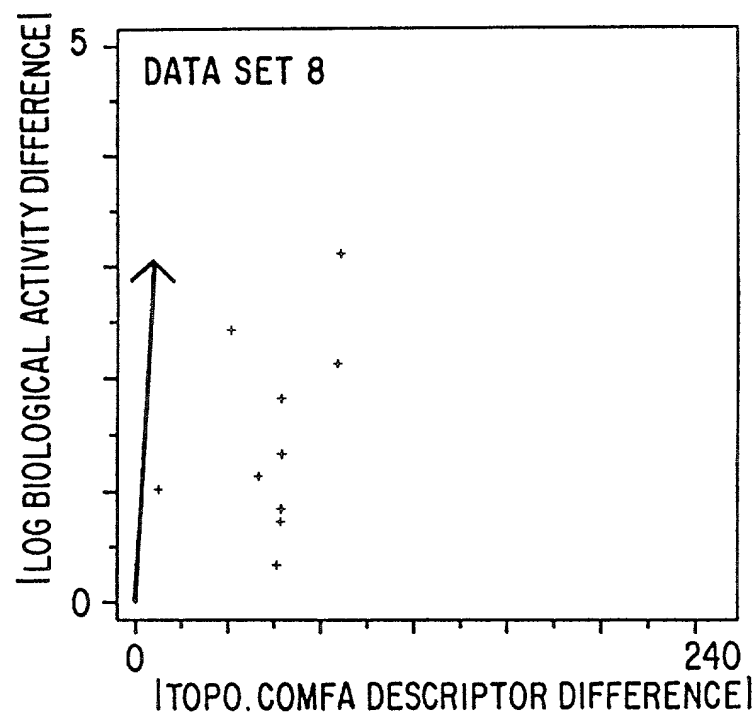


FIG.7(h)

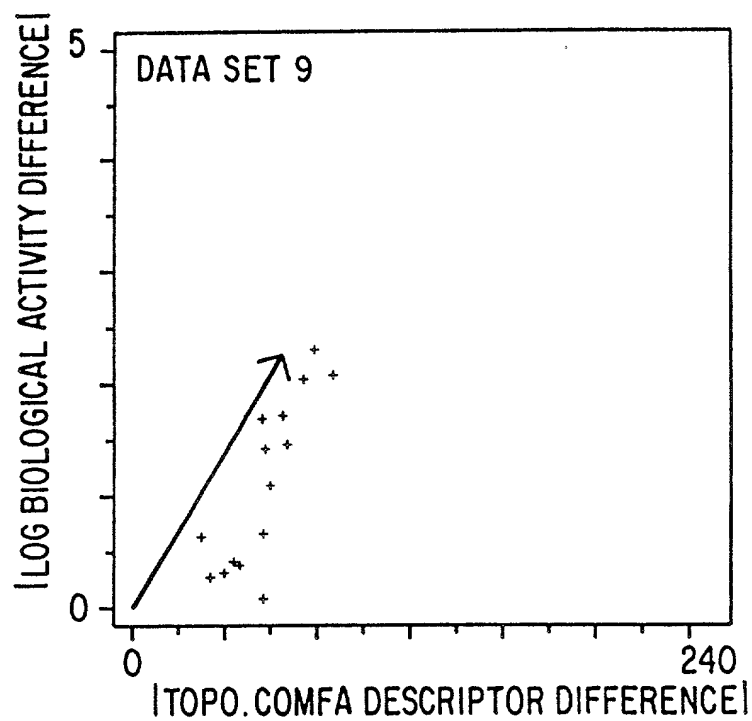


FIG.7(i)

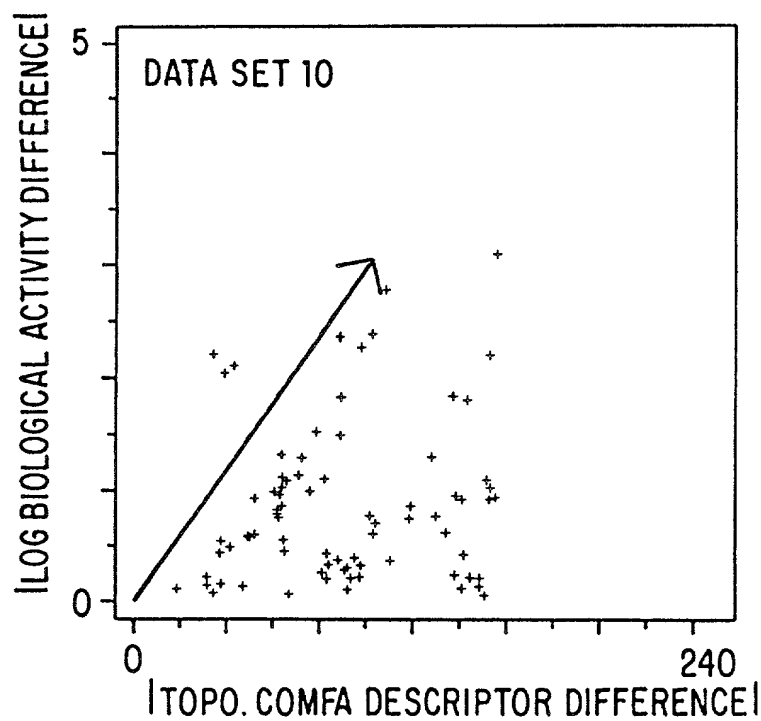


FIG.7(j)

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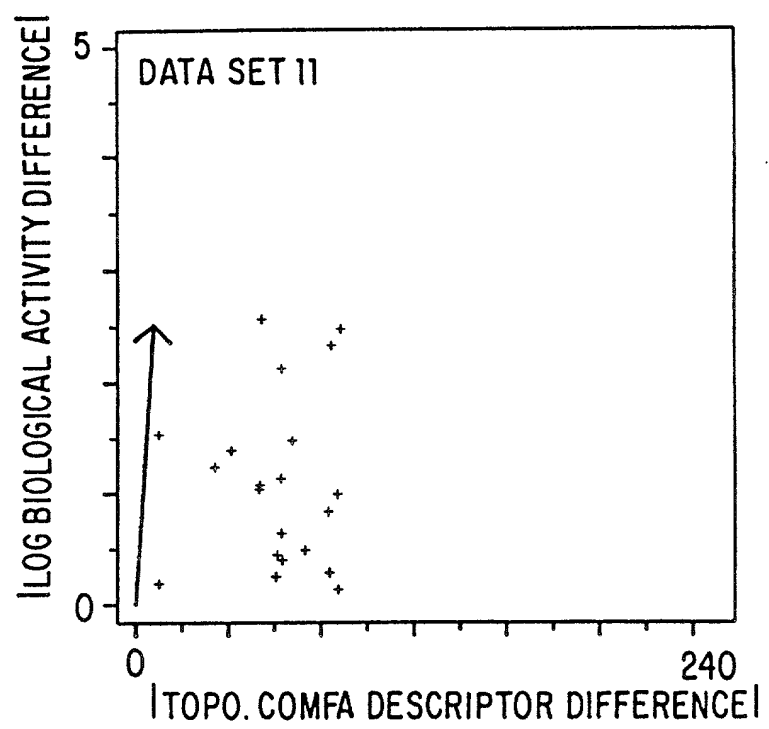


FIG.7(k)

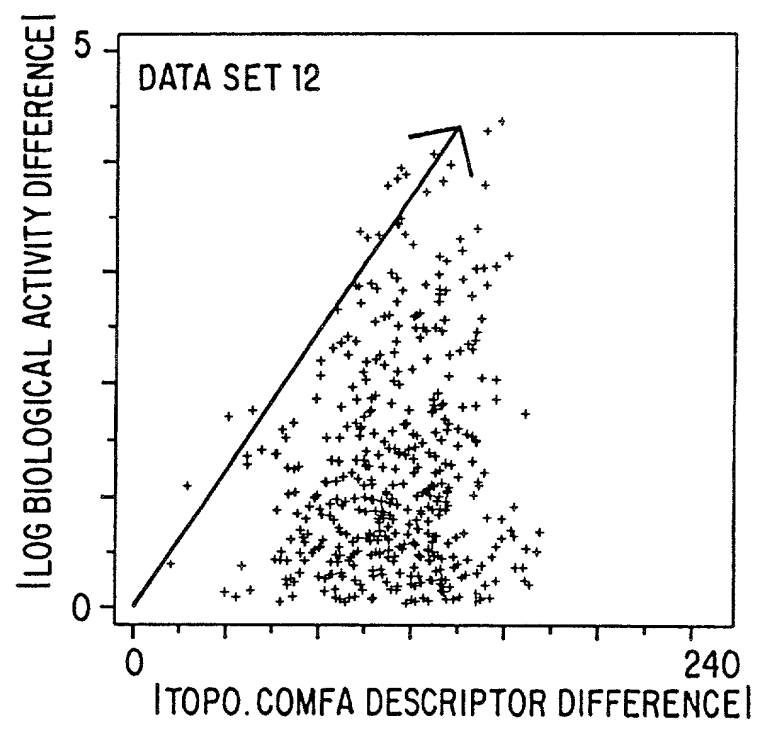


FIG.7(l)

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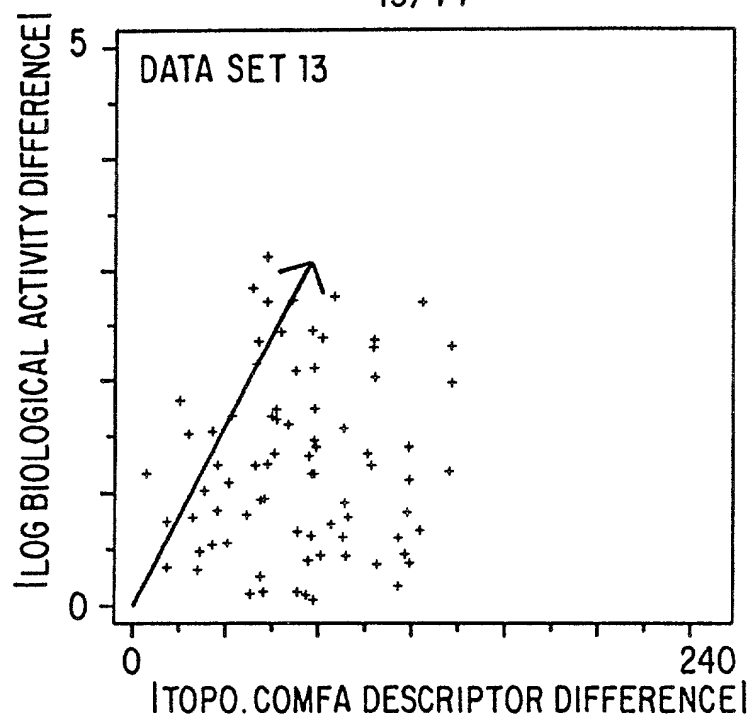


FIG.7(m)

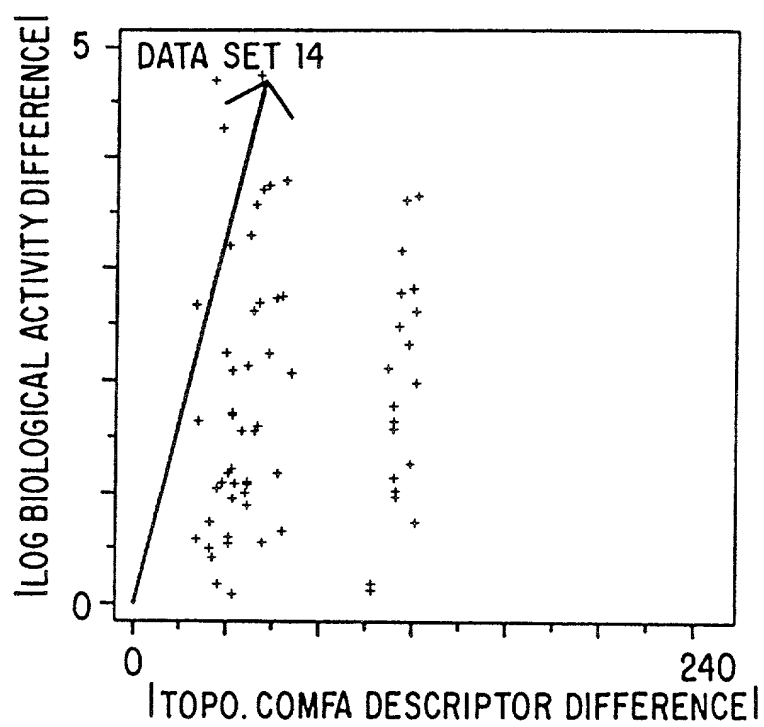


FIG.7(n)

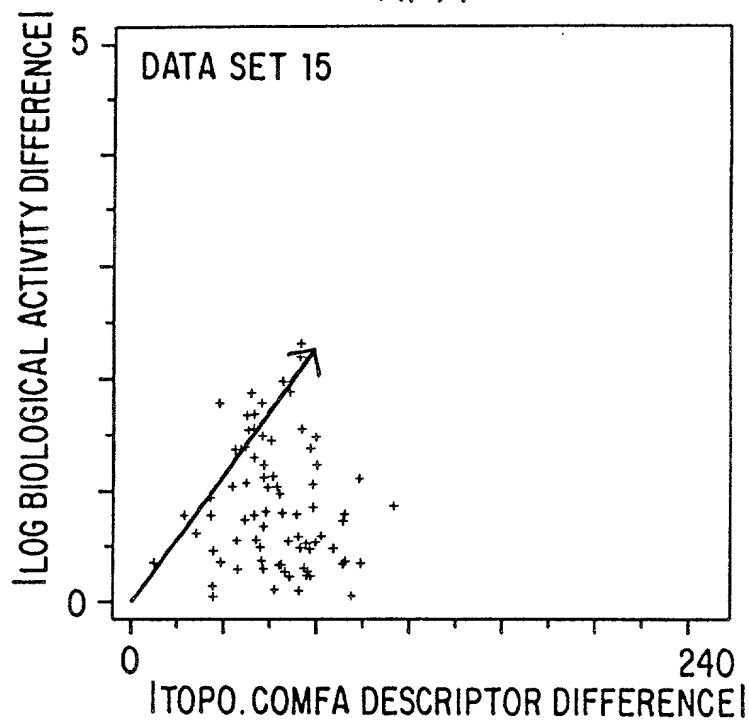


FIG.7(o)

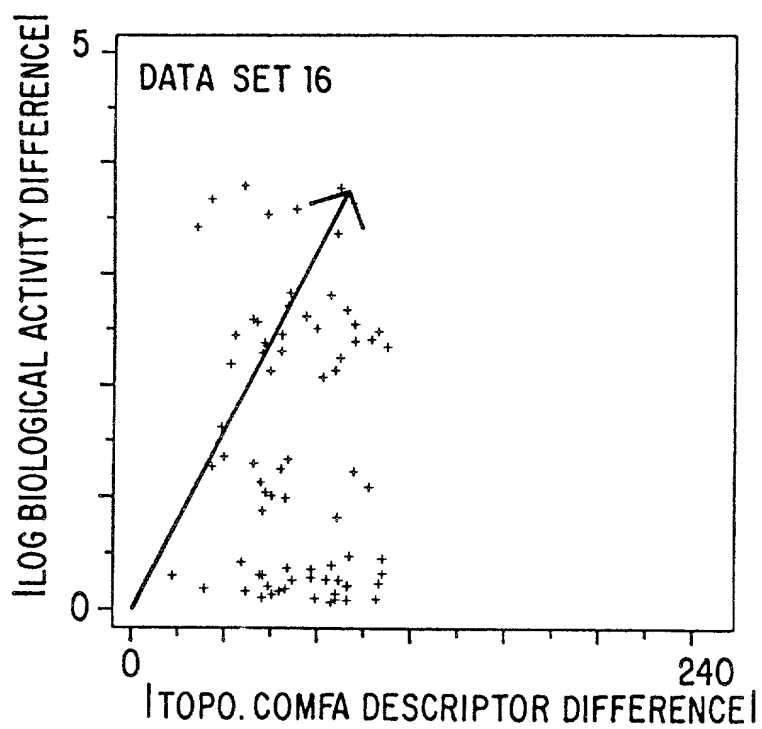


FIG. 7(p)

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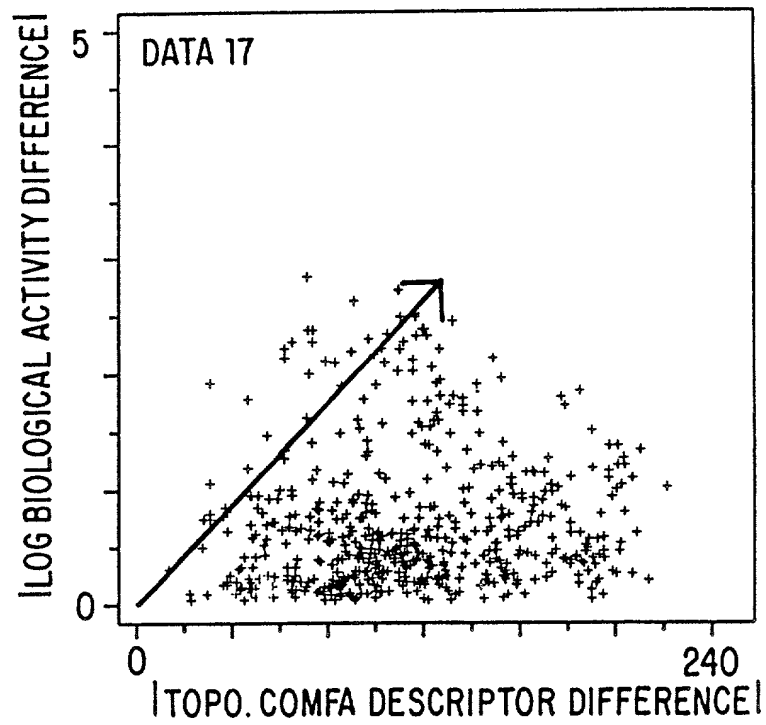


FIG.7(q)

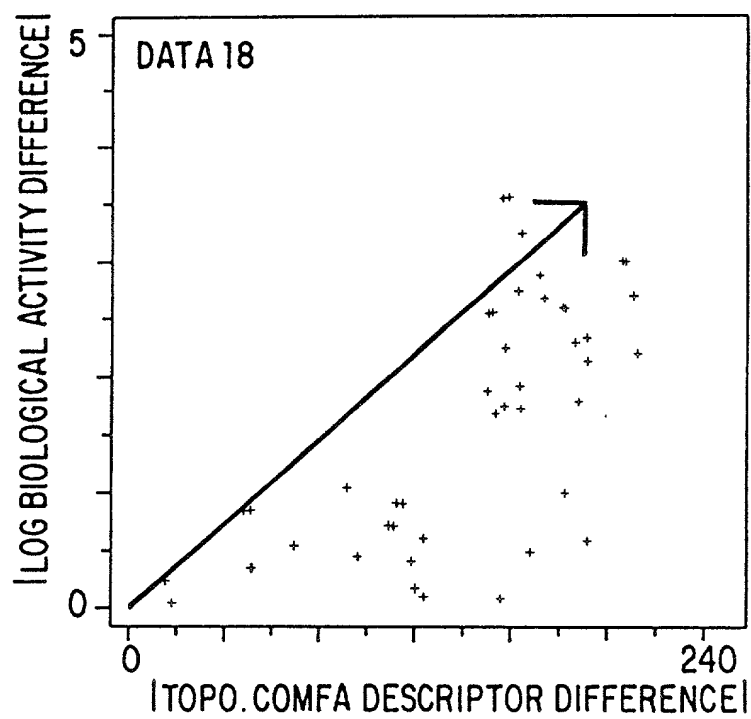


FIG.7(r)

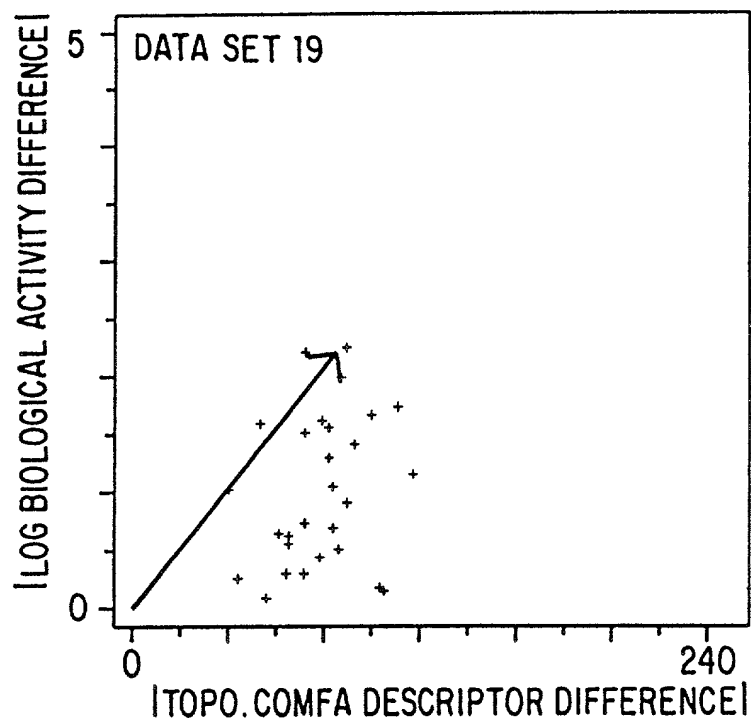


FIG. 7(s)

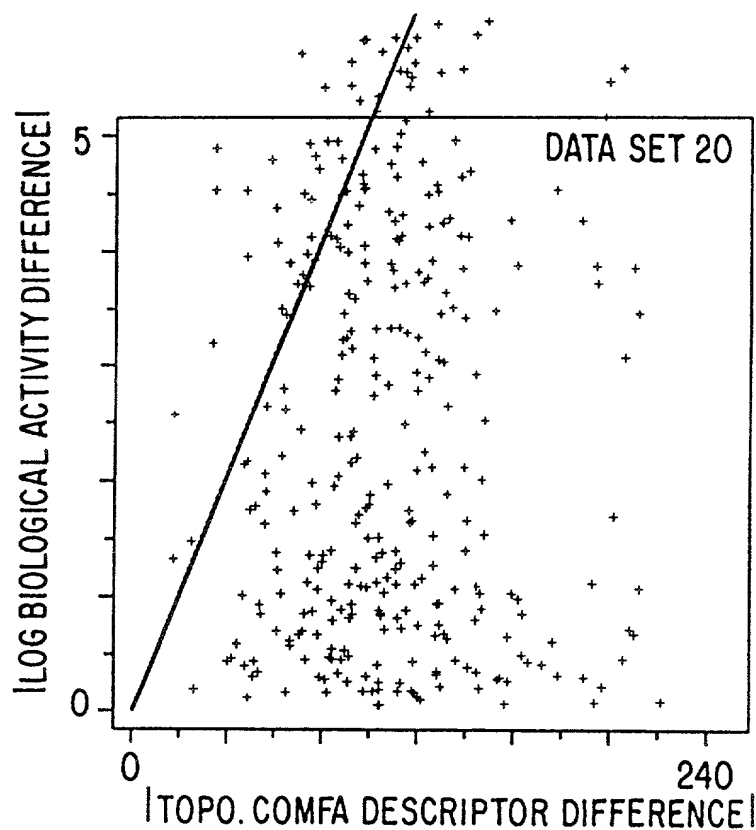
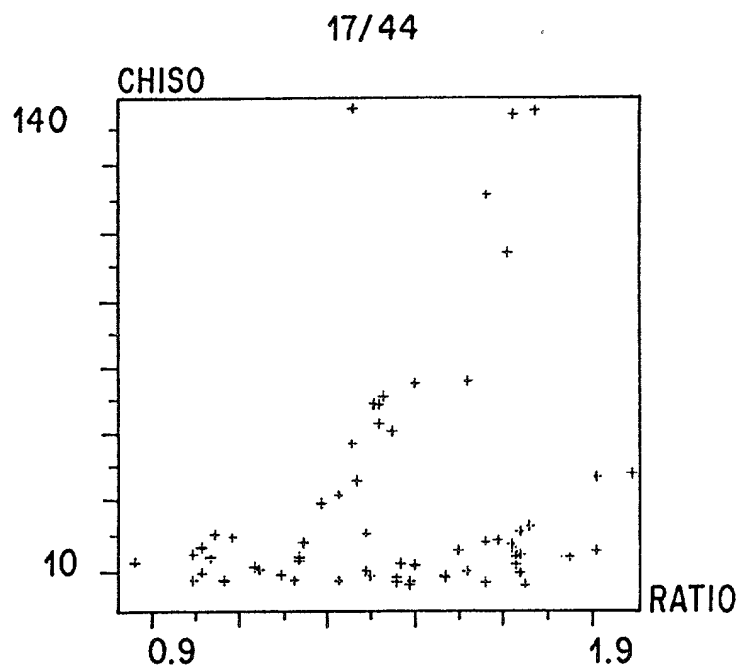


FIG. 7(t)



1.1

FIG. 8(a)

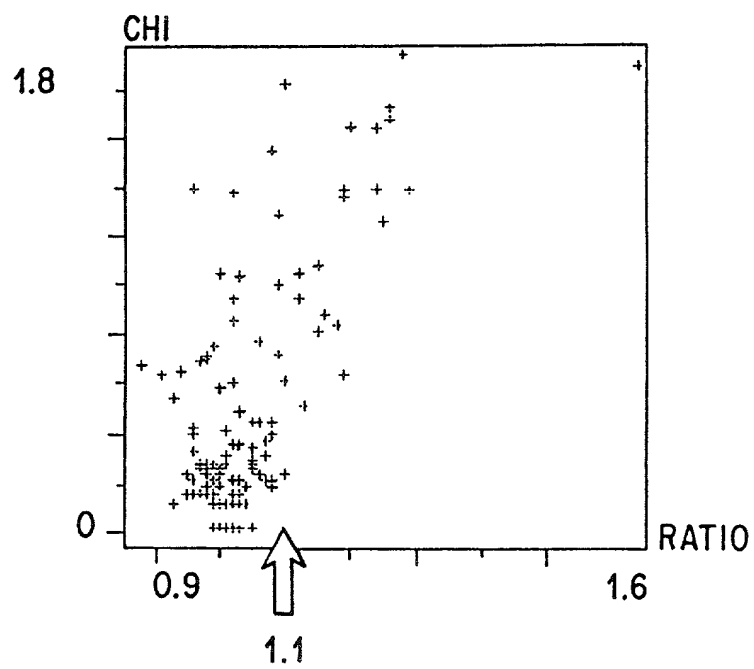


FIG. 8(b)

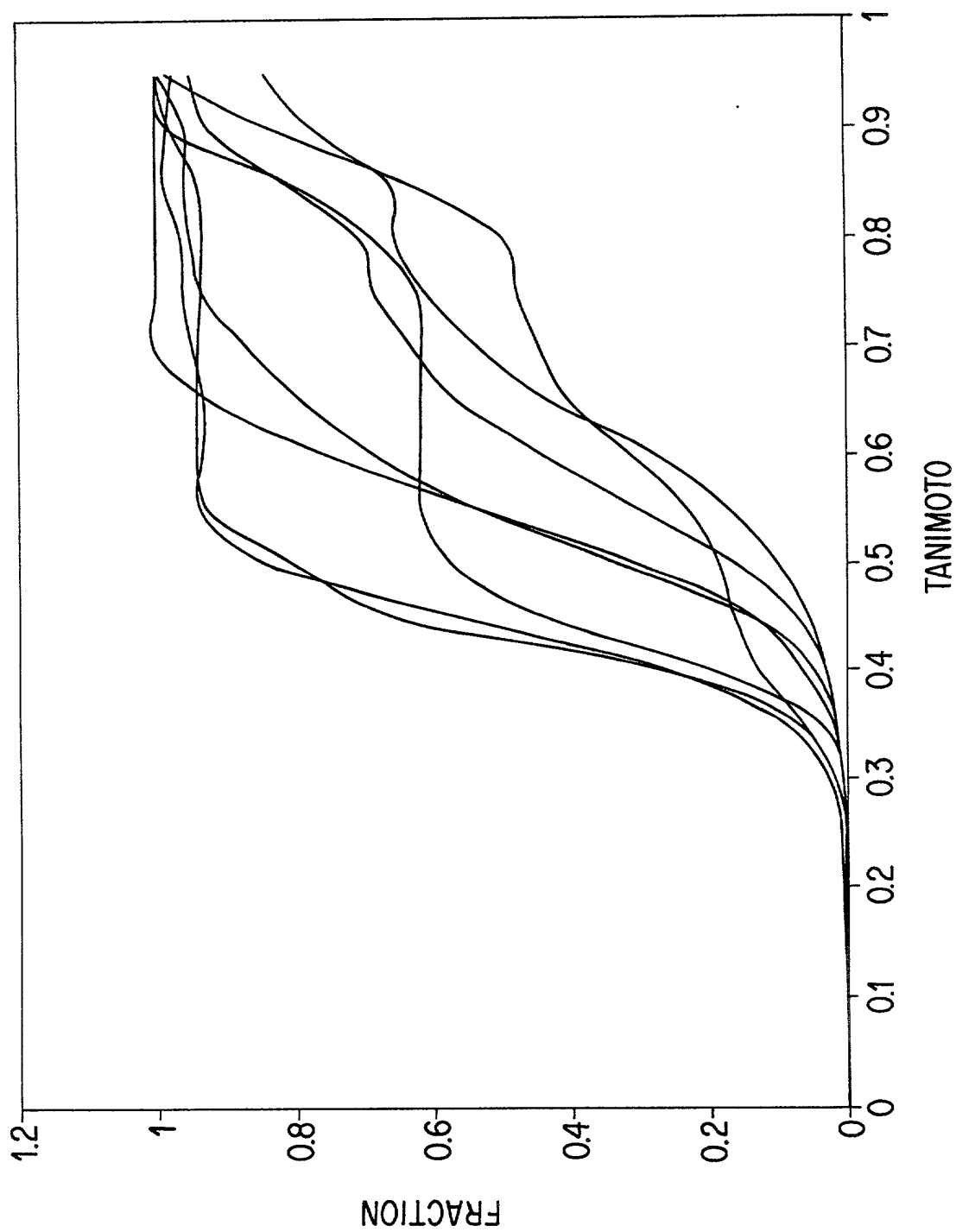


FIG. 9(a)

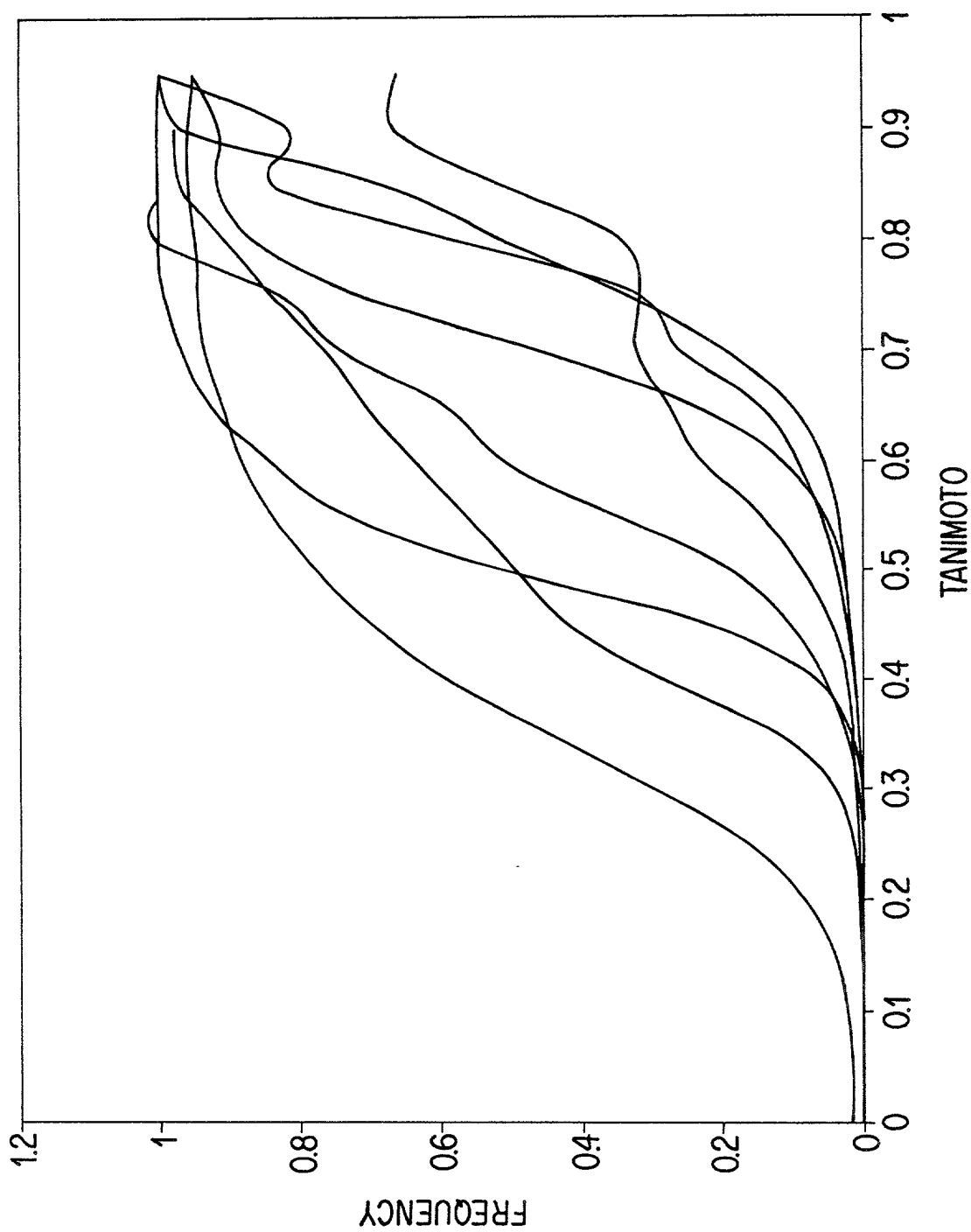
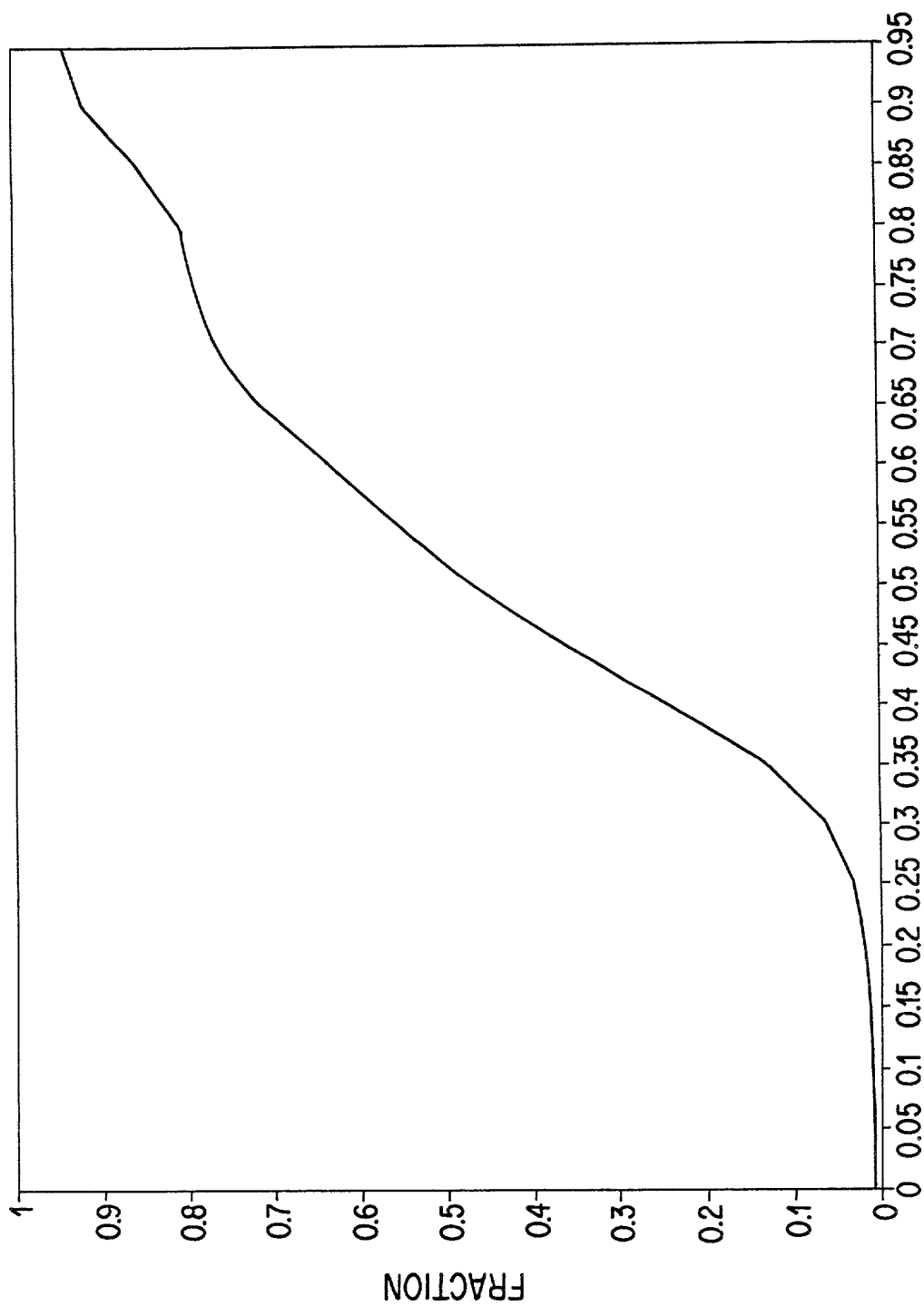


FIG. 9(b)



TANIMOTO

FIG. 9(c)

TOP-30" 55499360

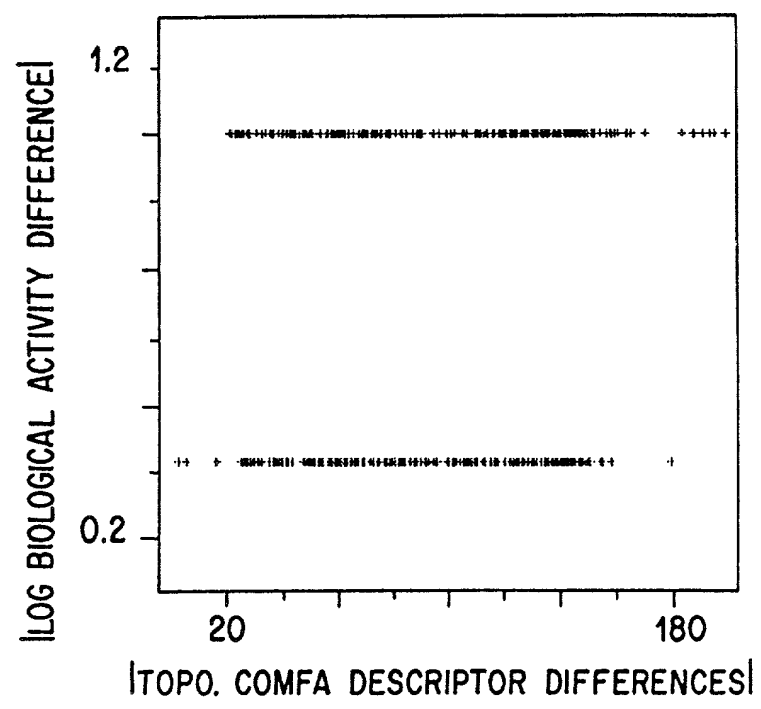


FIG.10(a)

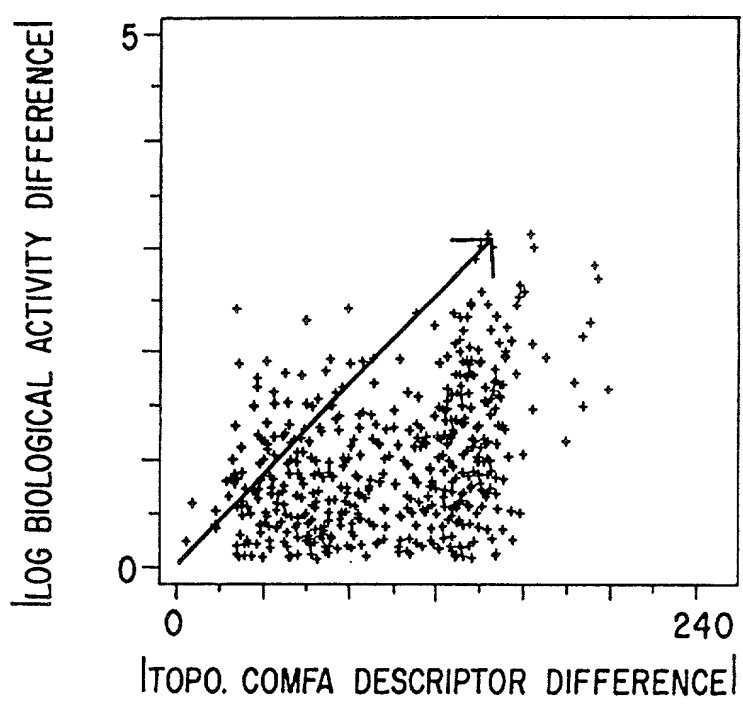


FIG.10(b)

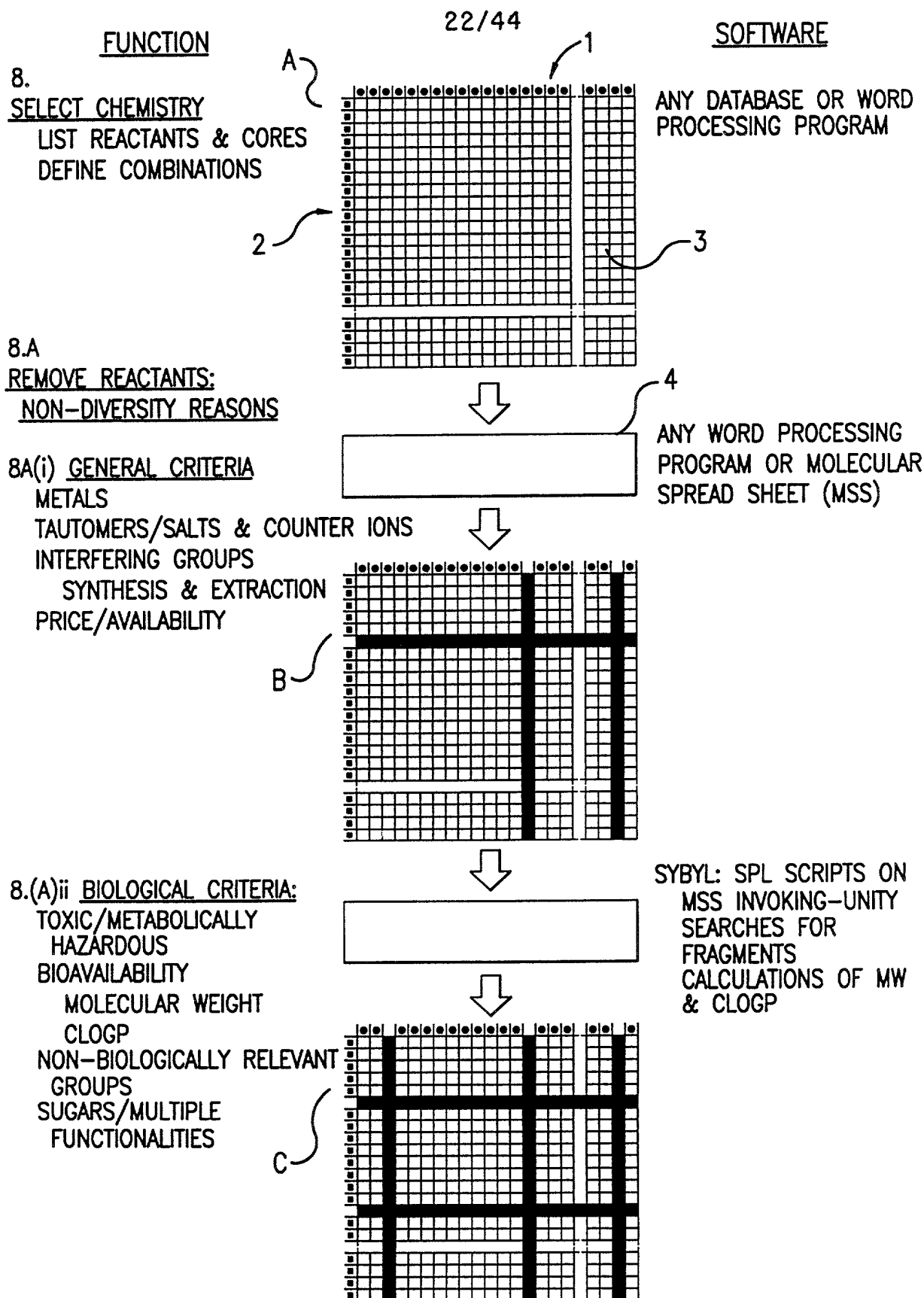


FIG.11(a)

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GENERAL INFORMATION

RIA:

RIA:

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TESTS

RIA:

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CTIC

END
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D
CTIC

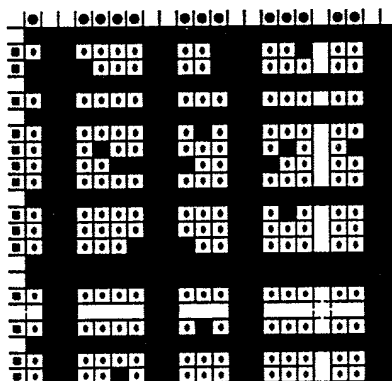
RIA:

8D

BIOLOGICAL CRITERIA:
 METABOLICALLY HAZARDOUS
 BIOAVAILABILITY
 MOLECULAR WEIGHT
 CLOGP

SYBYL: SPL SCRIPTS ON
 MSS INVOKING -
 UNITY SEARCHES FOR
 FRAGMENTS
 CALCULATIONS OF MW
 & CLOGP

G



8E

REMOVE NON-DIVERSE
 PRODUCTS:

GENERATE TANIMOTO
 2D FINGERPRINTS
 SAMPLE PRODUCTS:
 EXCLUDE TAN ≥ 0.85

UNITY

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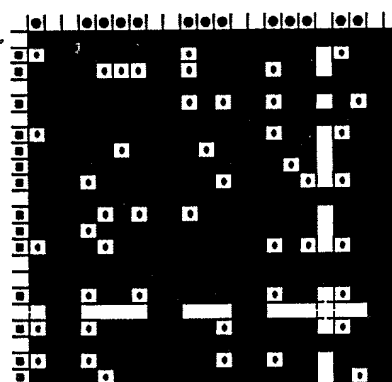
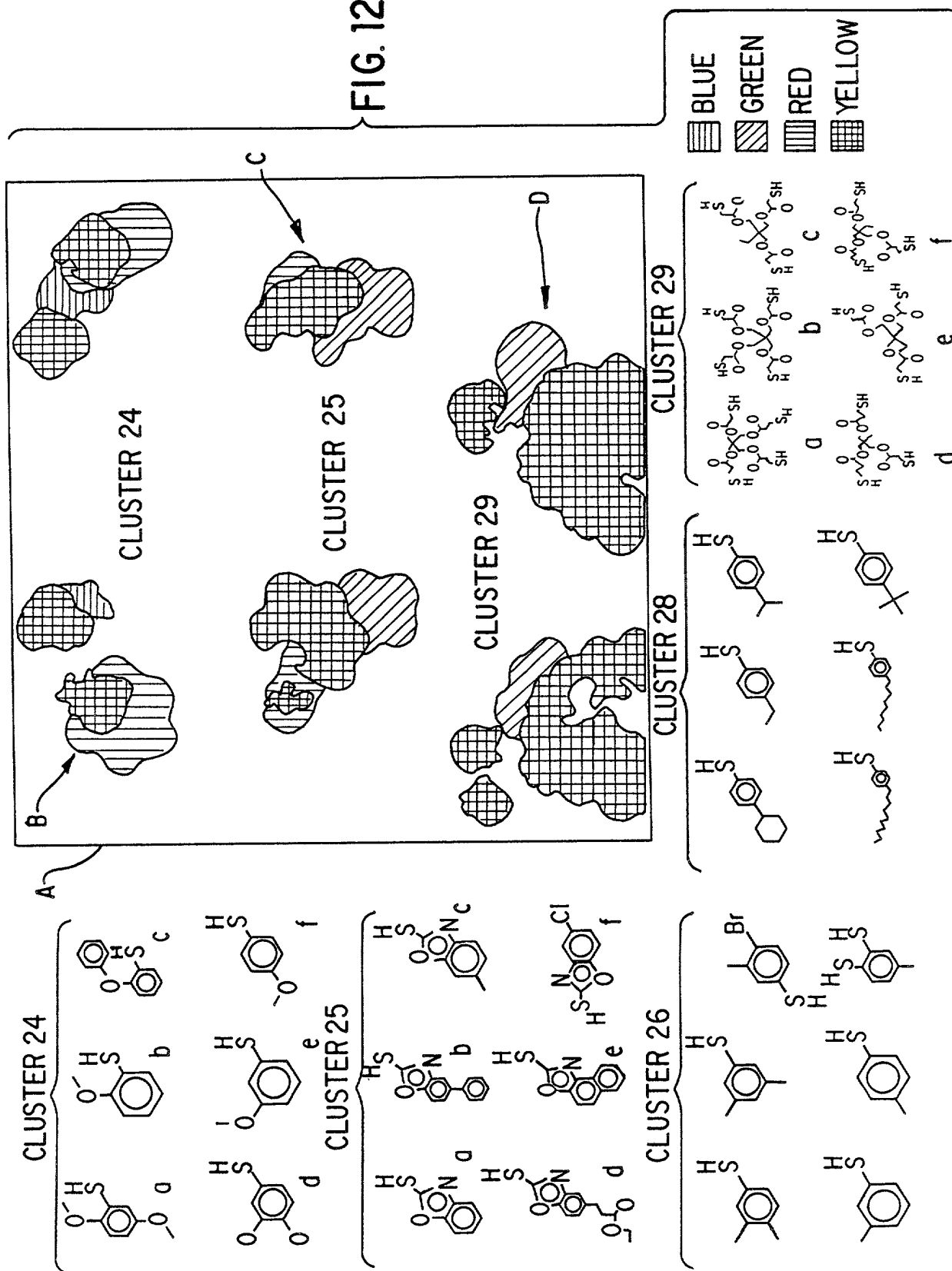


FIG.11(c)

FIG. 12



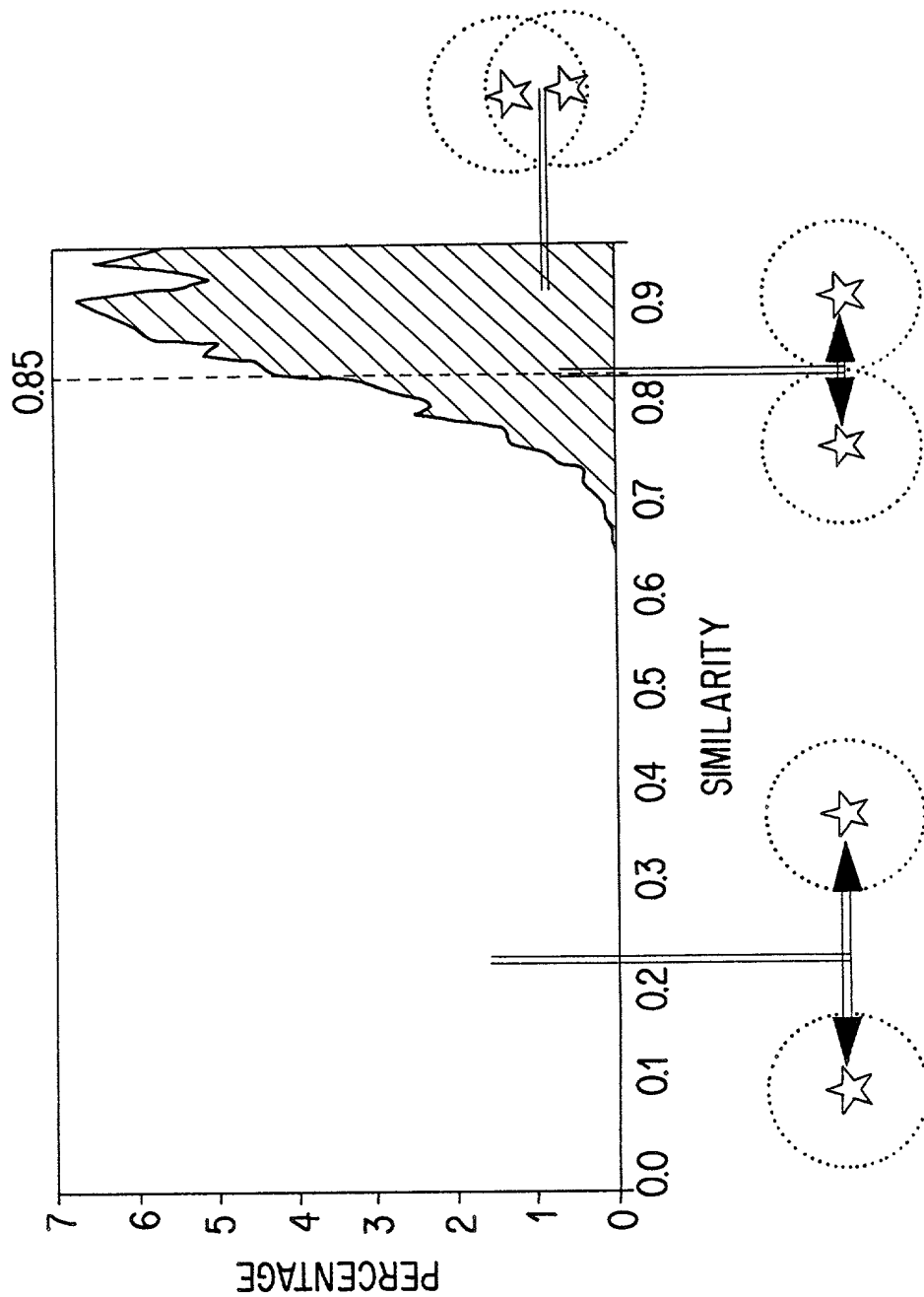


FIG.13

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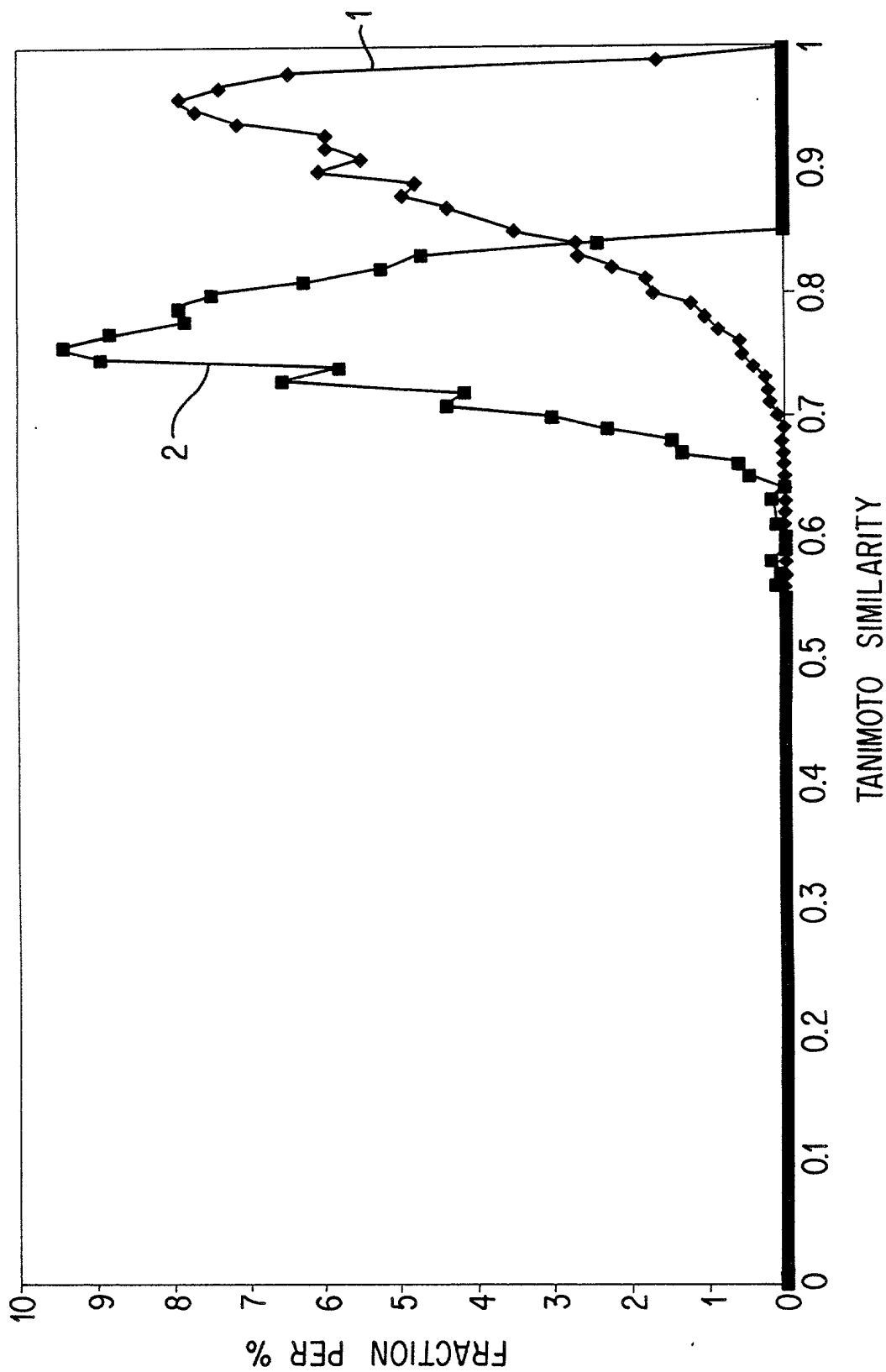


FIG.14

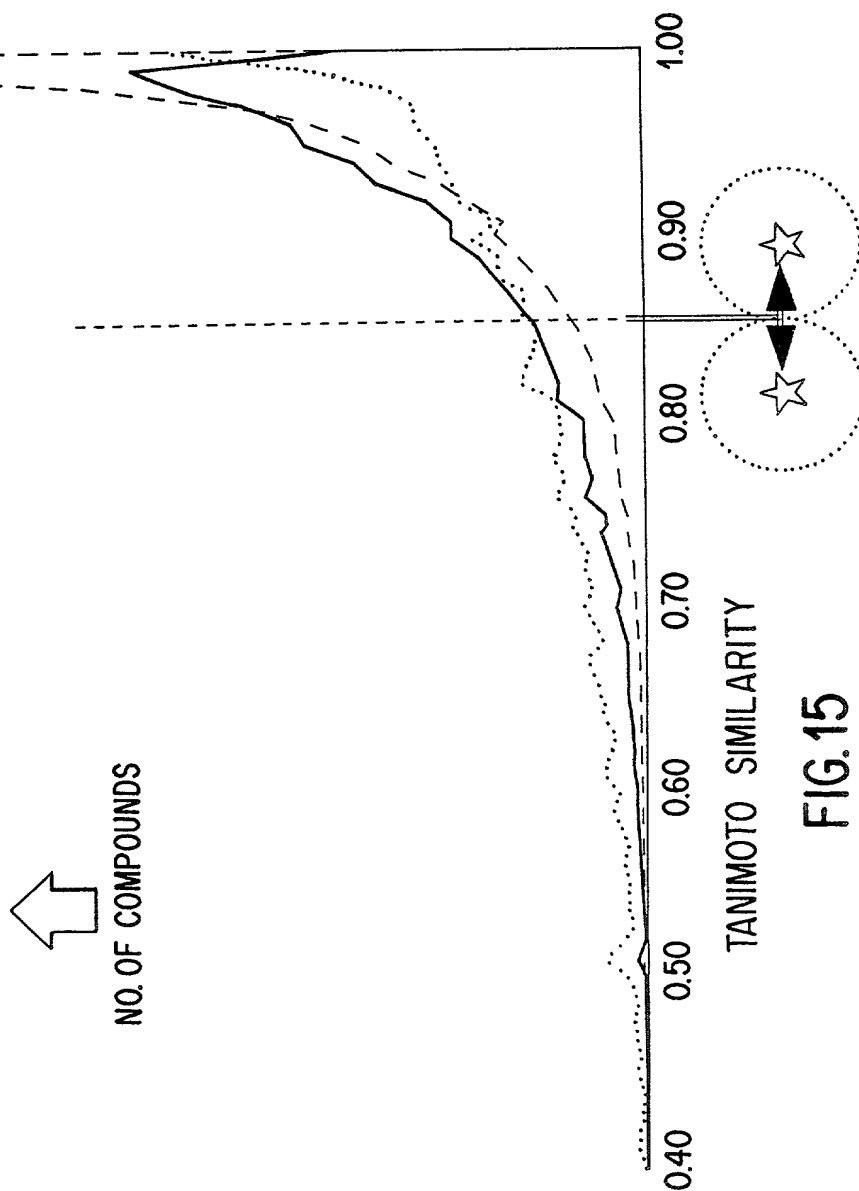


FIG.15

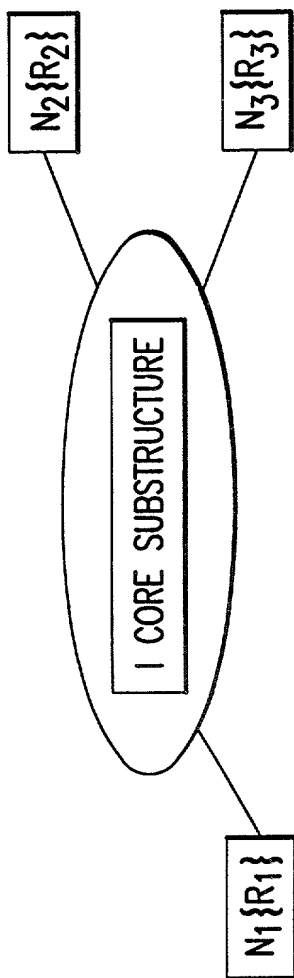


FIG.16

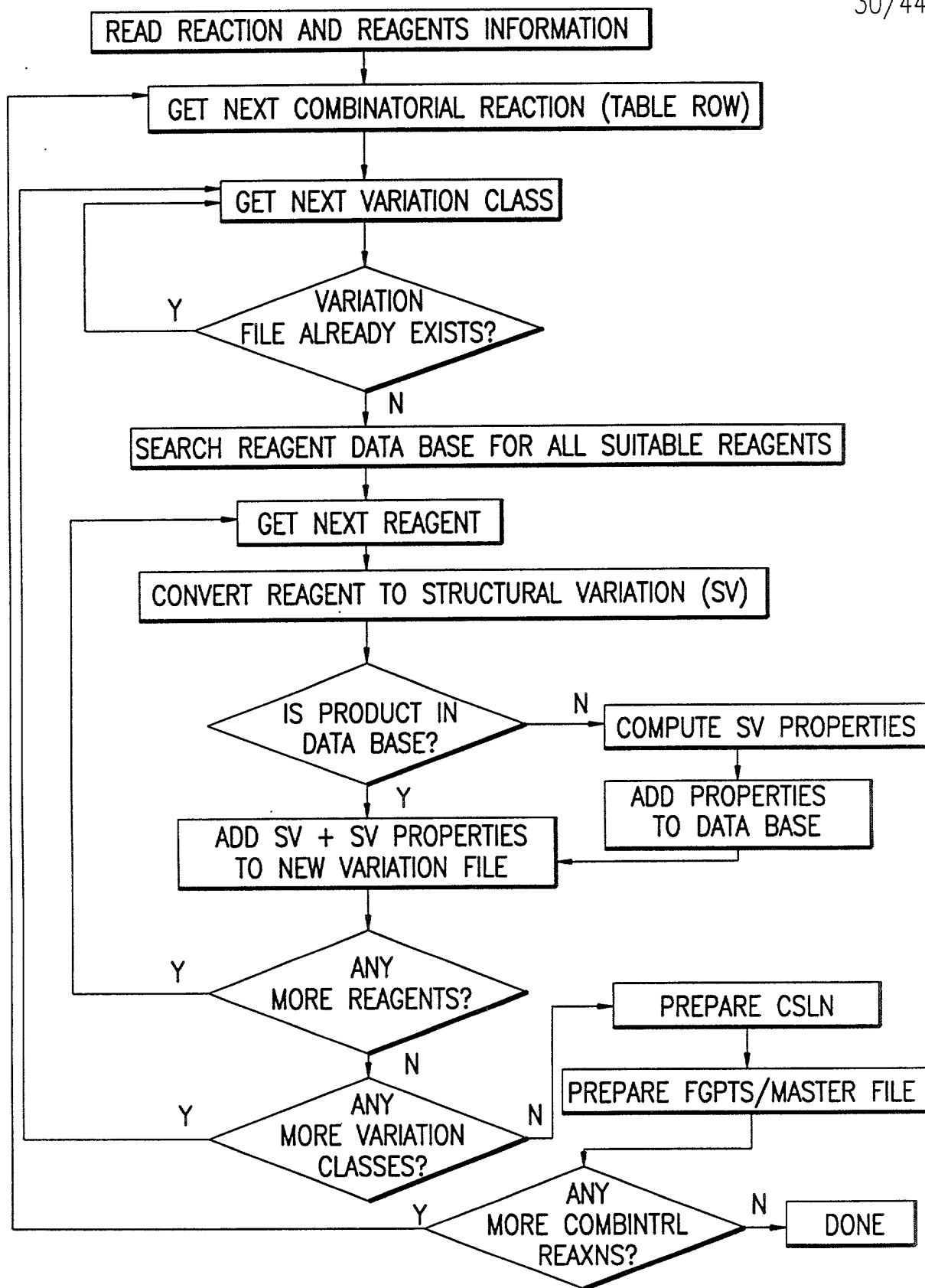


FIG.17

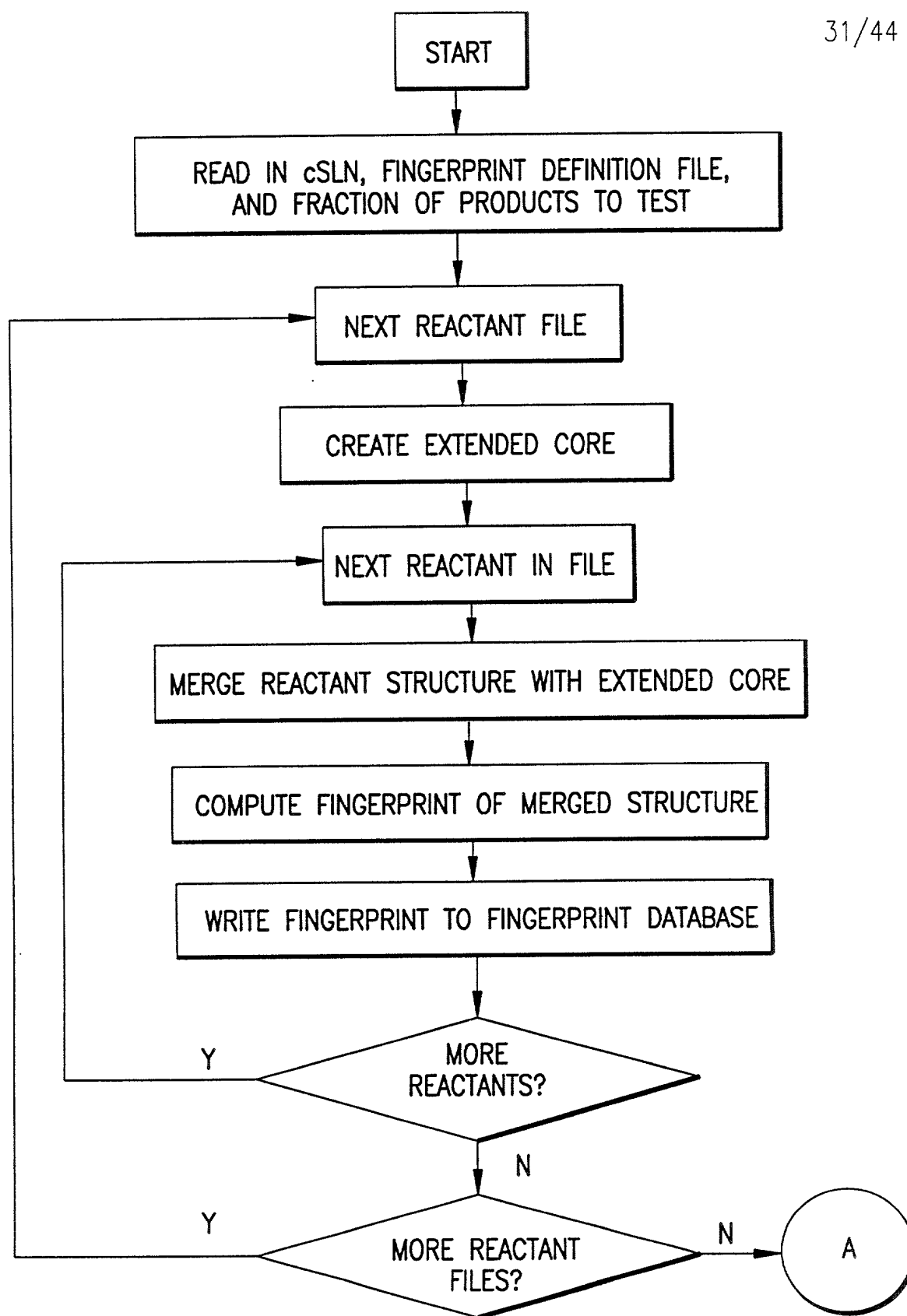


FIG.18

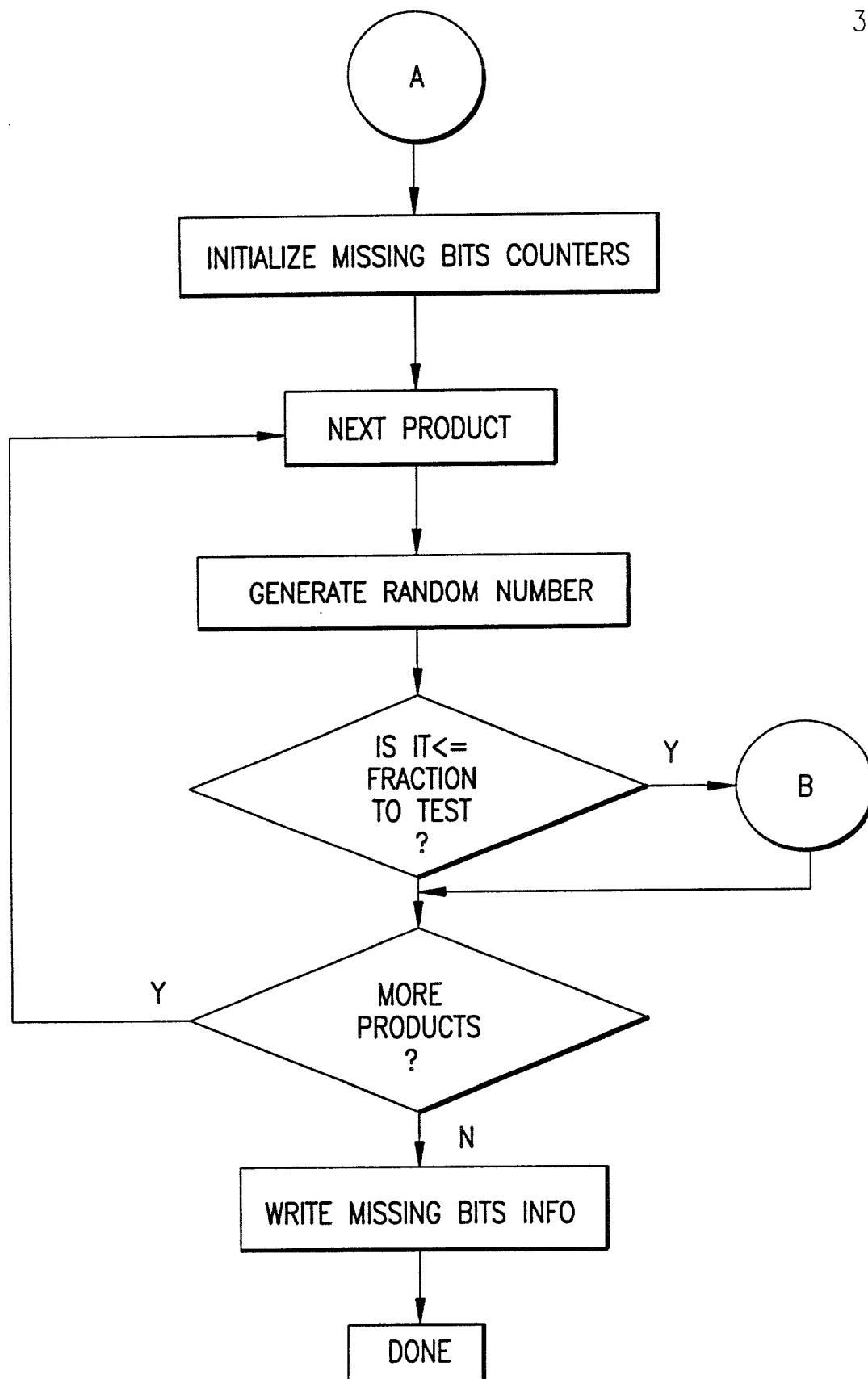


FIG.19

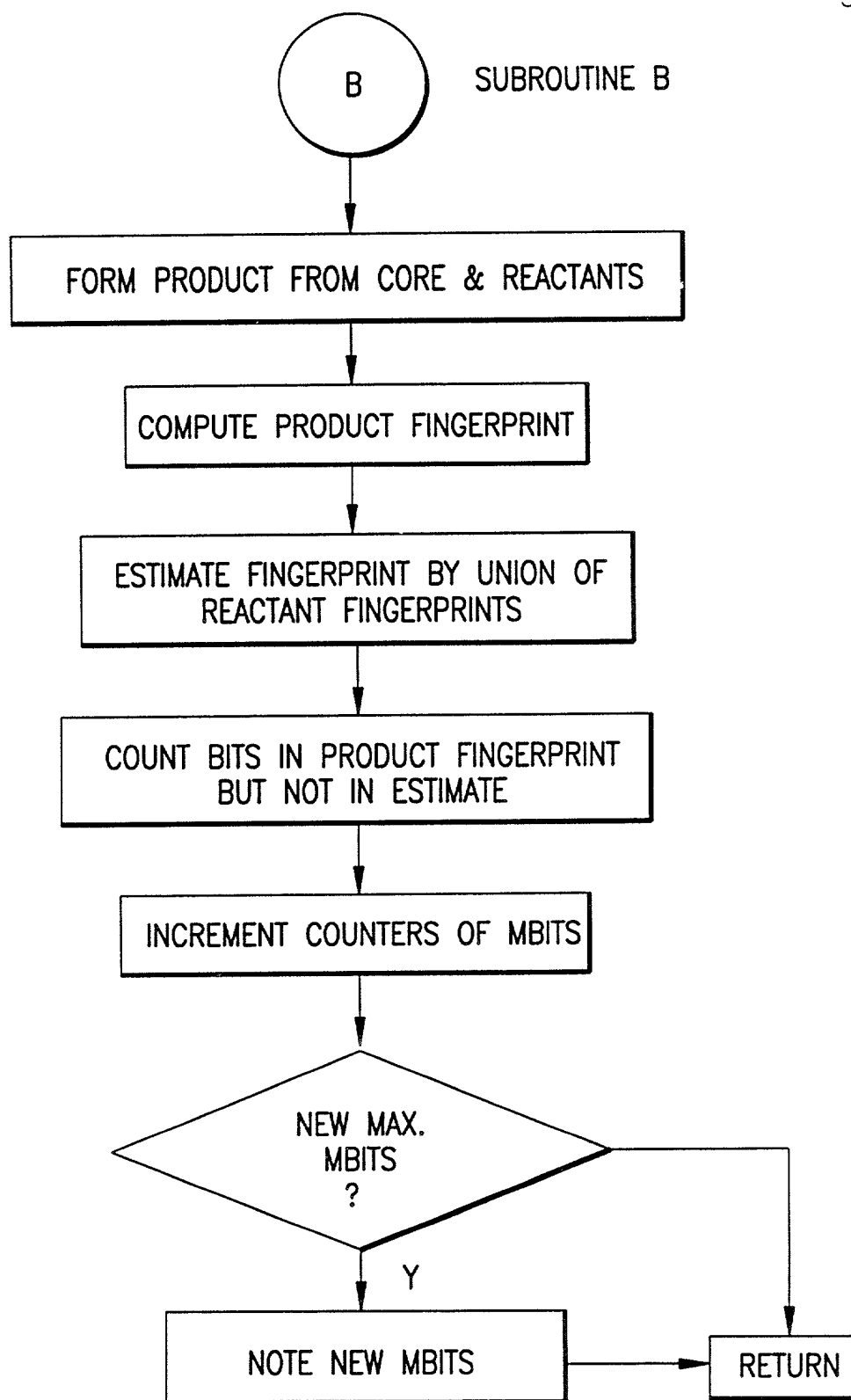


FIG.20

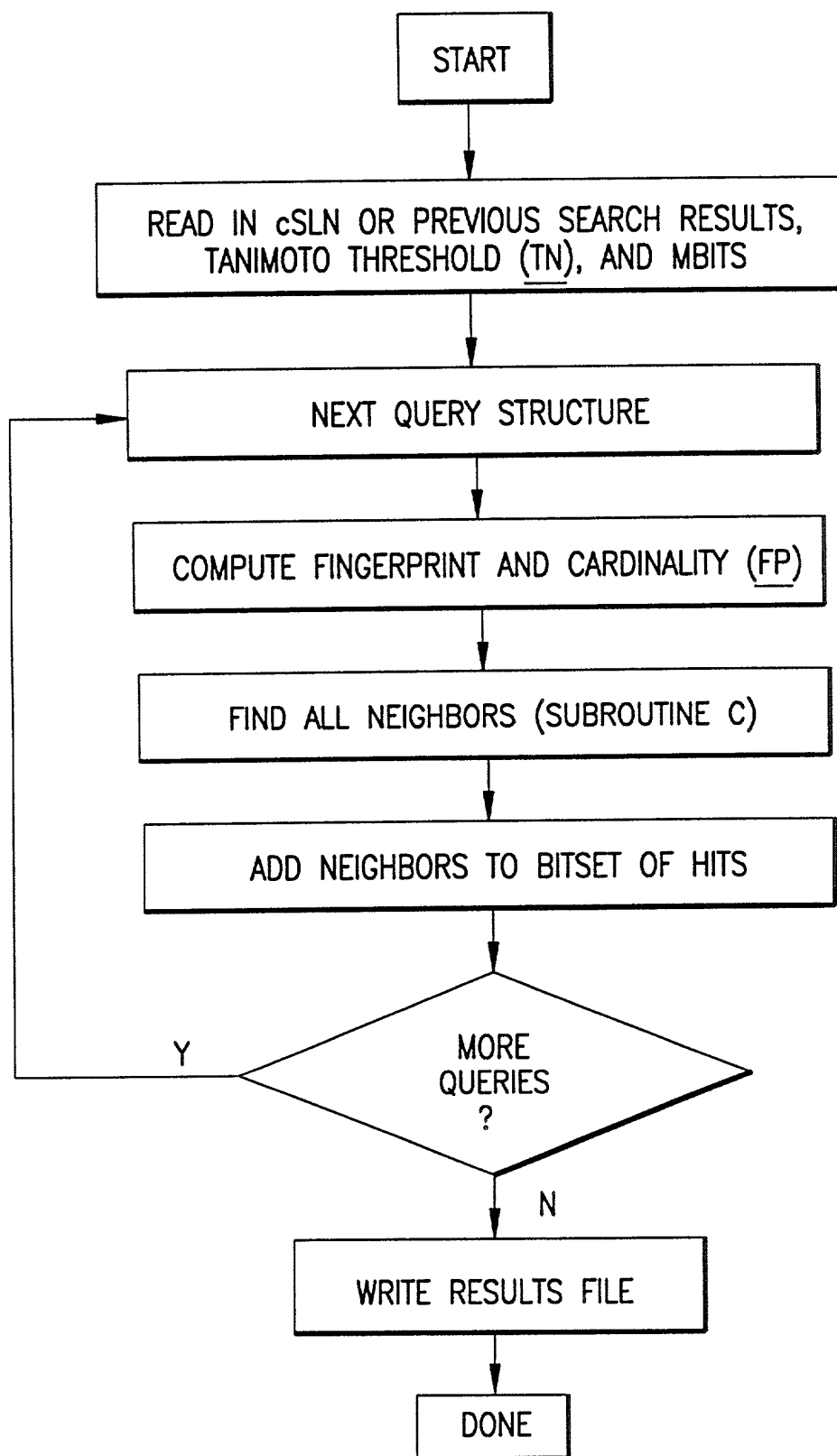
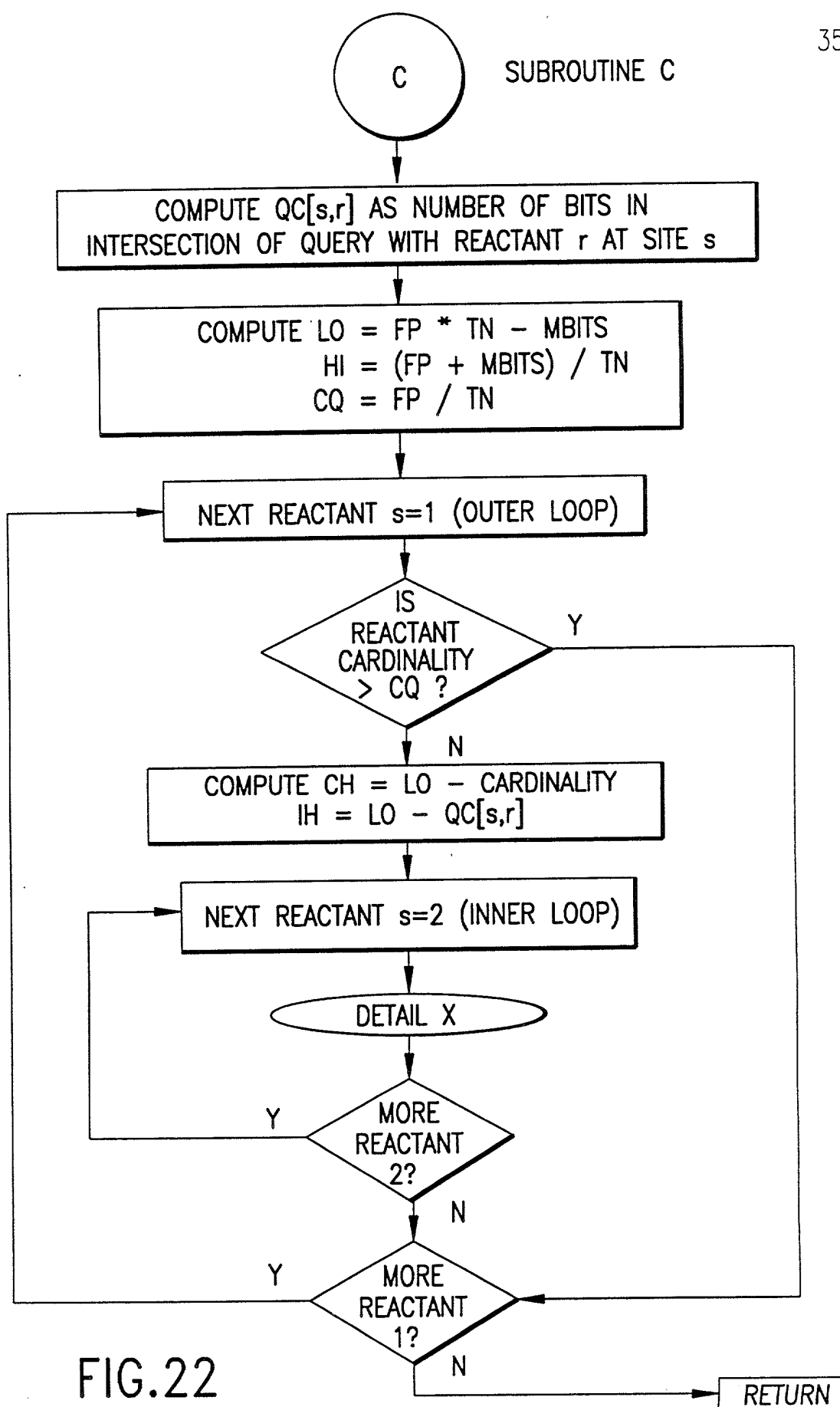


FIG.21



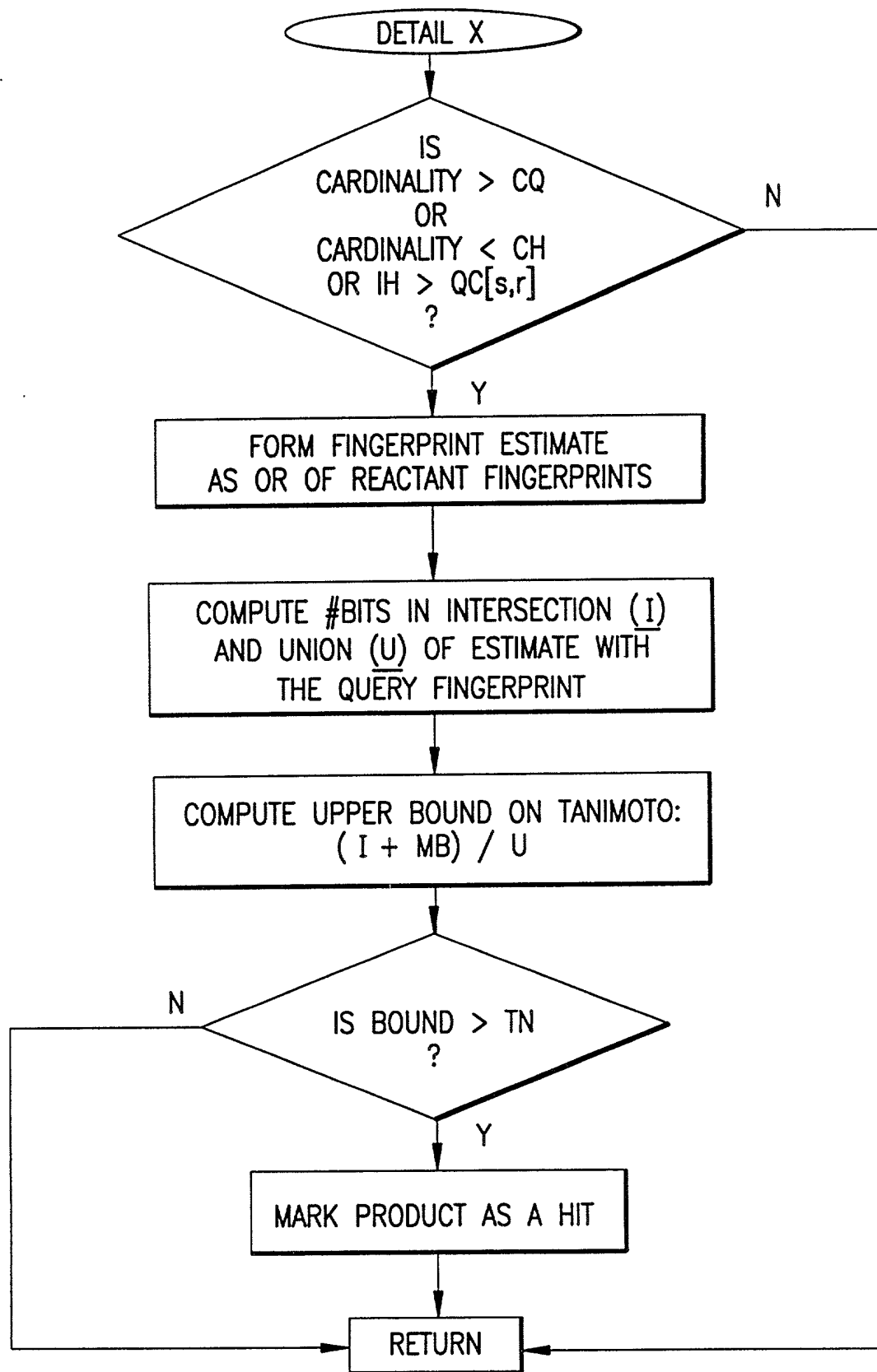


FIG.23

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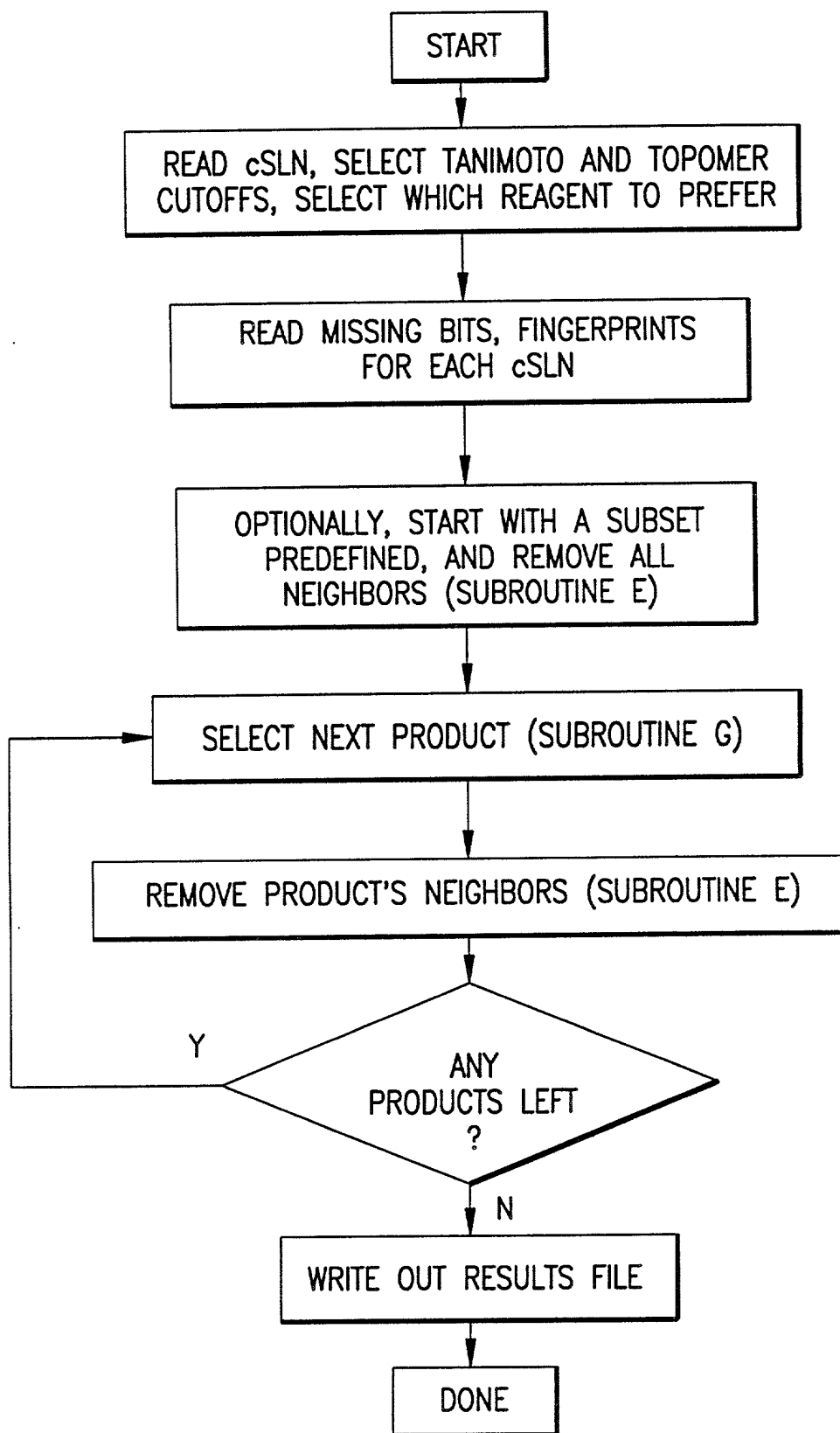


FIG.24



FIG.25

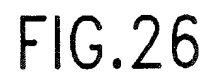


FIG.26

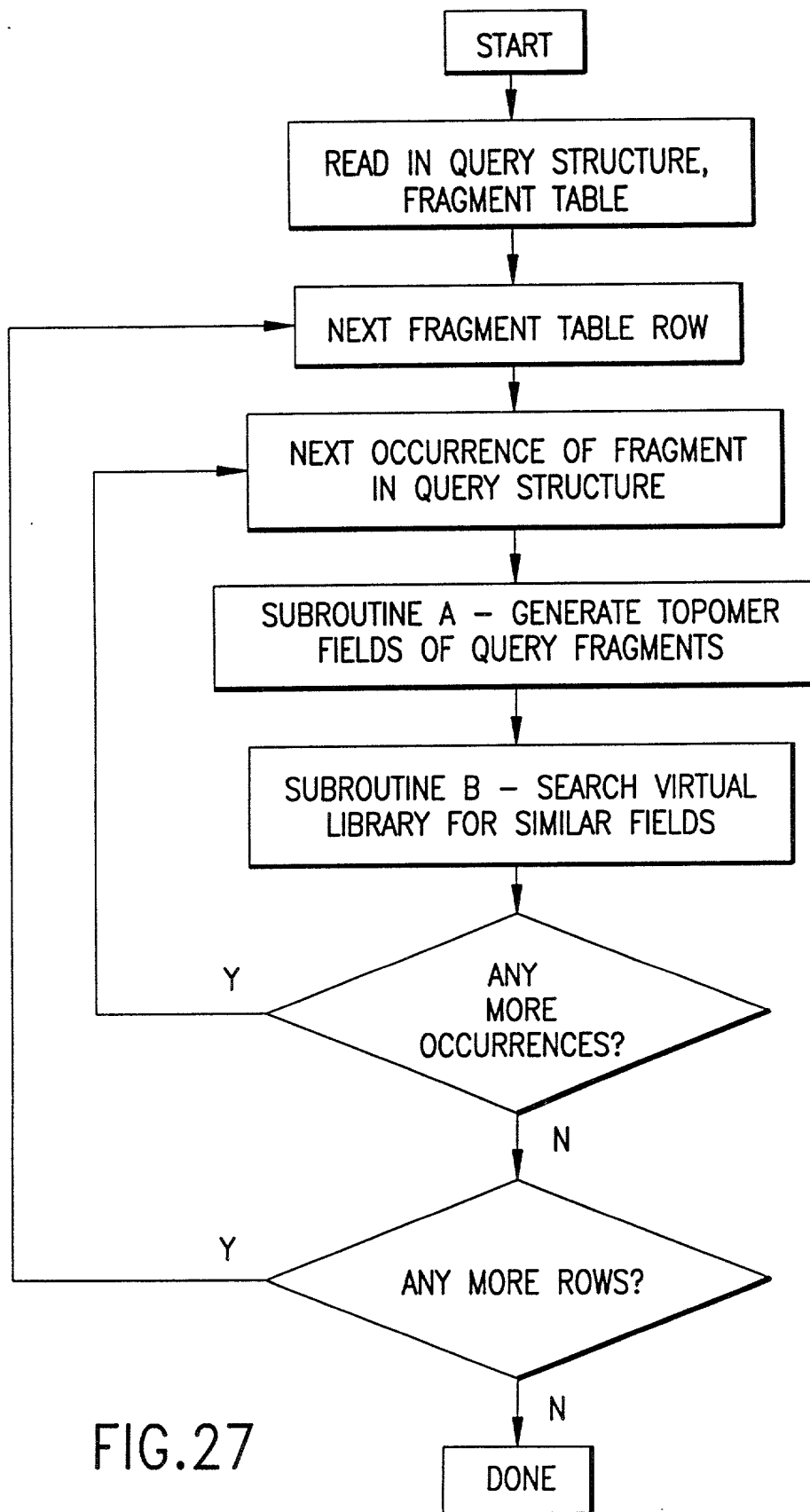


FIG.27

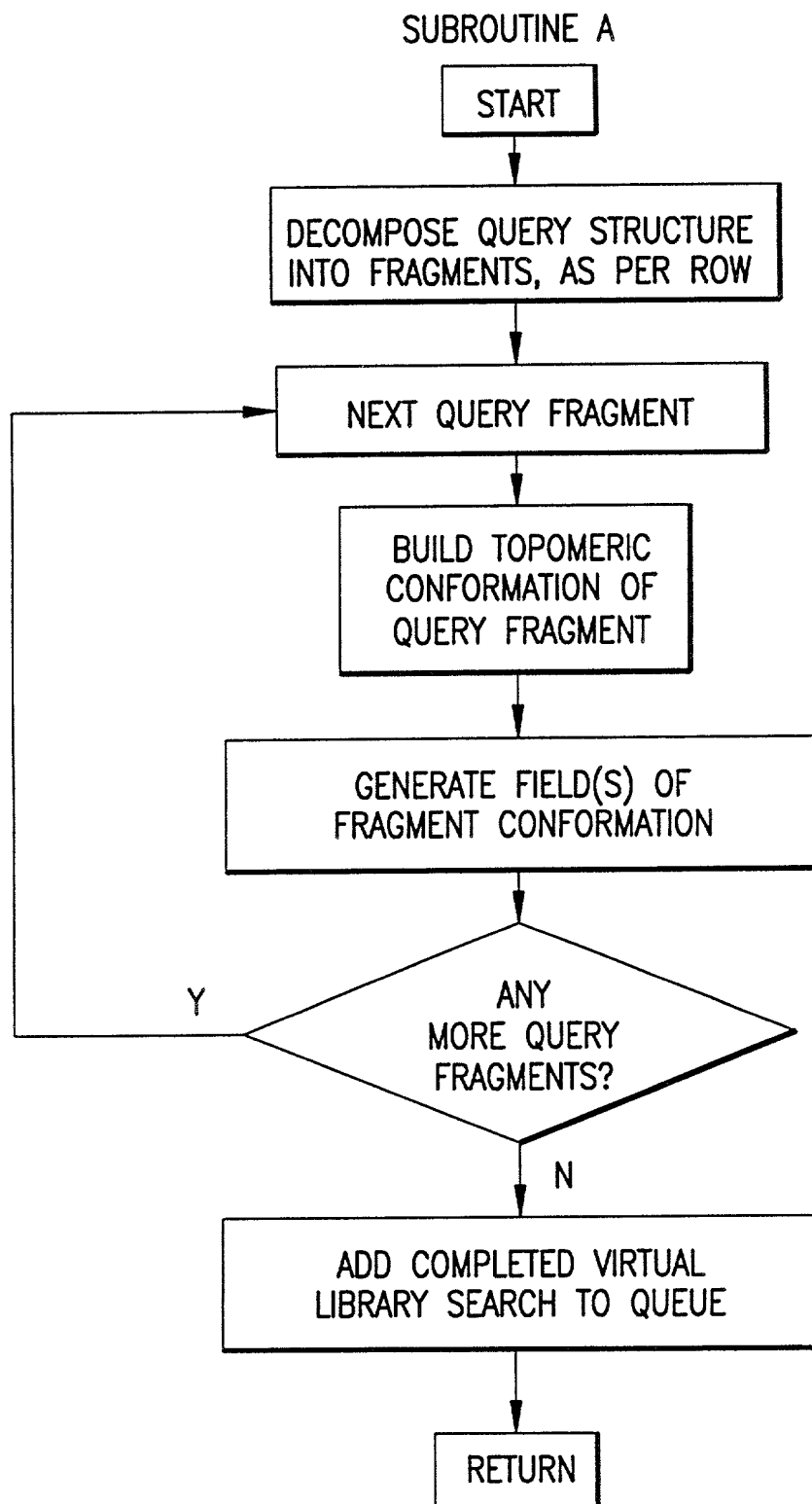


FIG.28

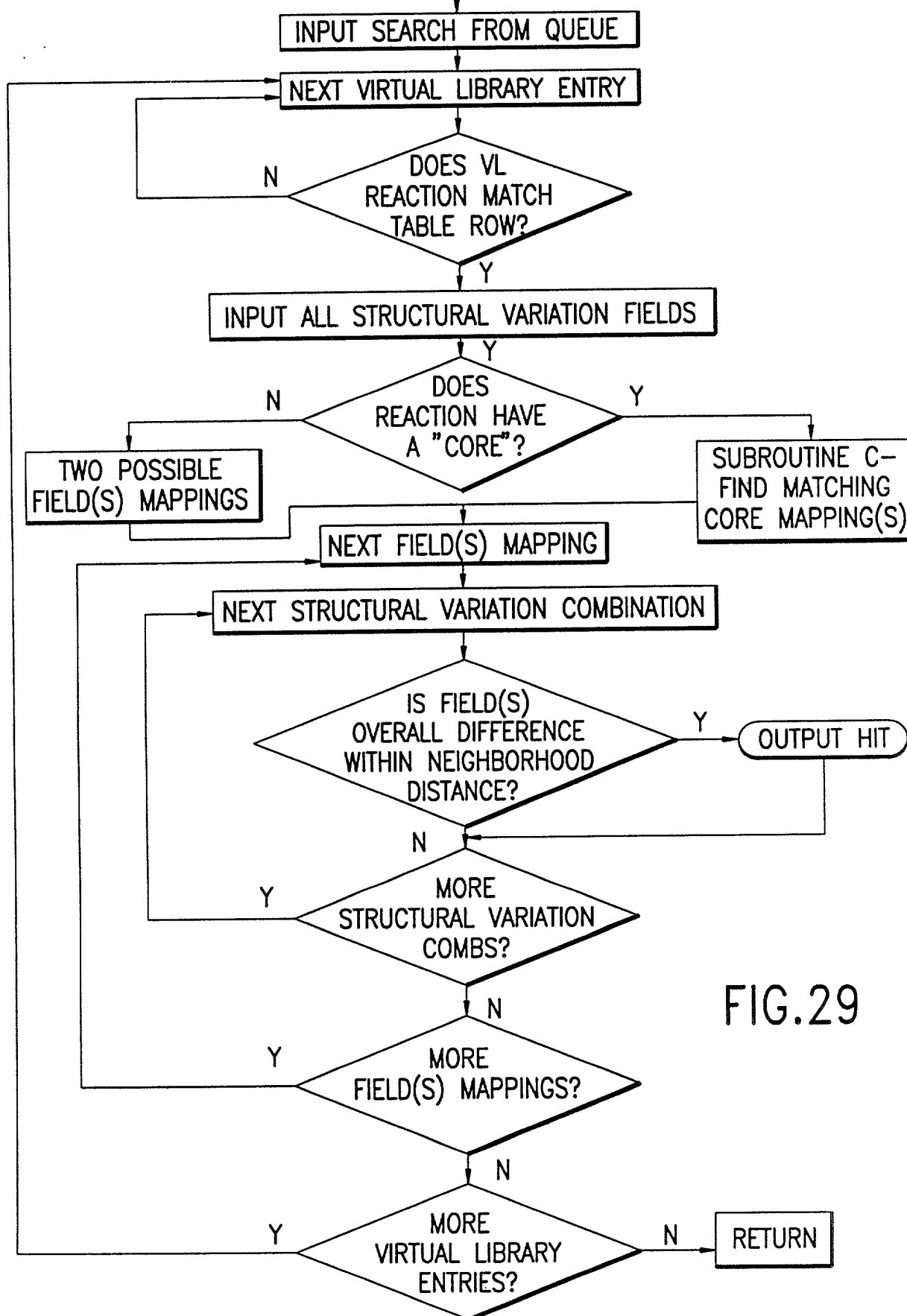


FIG.29

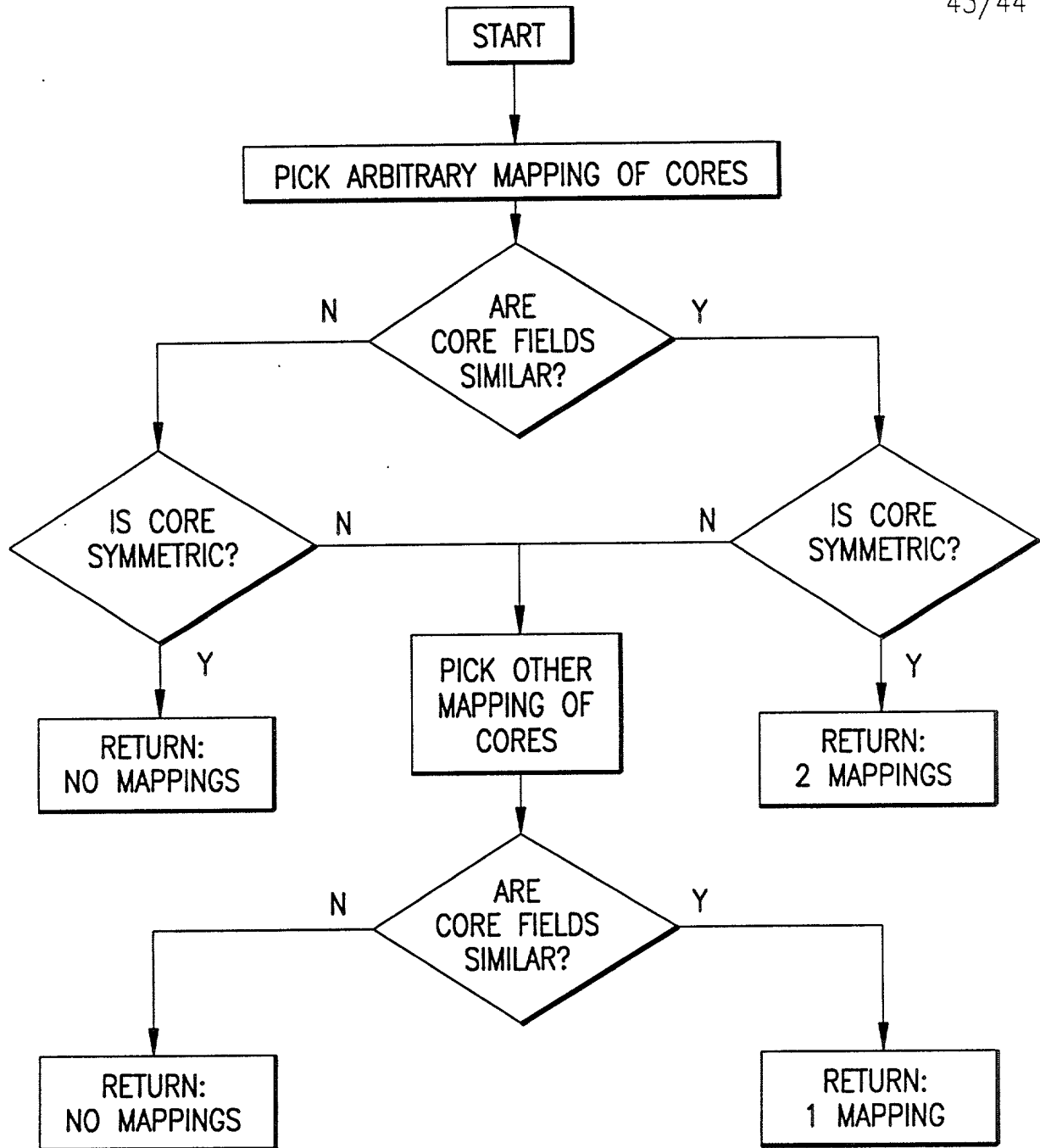


FIG.30

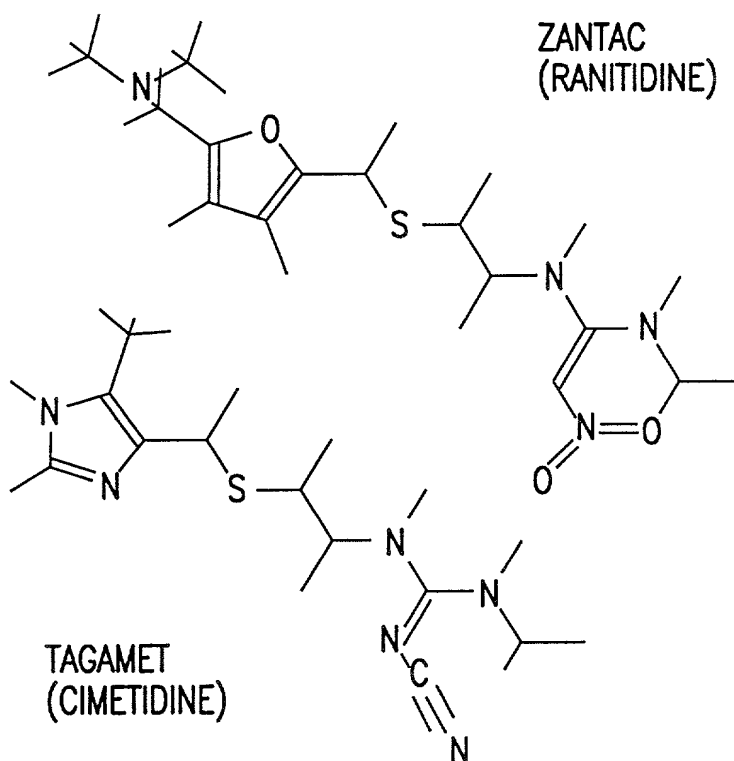
[illegible]

FIG.31